Analytical models of electron leakage currents in gallium nitride-based laser diodes and light-emitting diodes: supplement

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Analytical models of electron leakage currents in gallium nitride-based laser diodes and light-emitting diodes: supplemental document

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1. Band structures and the equivalent circuits of the LDs

In the main text, we have treated the electron-hole system as a parallel circuit and replace the increments of the quasi-Fermi level drop with the increments of the real voltage drop in Eq. (7). The assumption relies on the fact that the increments of \((E_c - E_{fn})\) or \((E_p - E_{fp})\) at boundaries, determining the increments of the carrier concentration, are relatively small compared to the increments of the total Fermi level drops on the whole p area, where \(E_c / E_v\) is the conduction/valance band and \(E_{fn} / E_{fp}\) is the quasi-Fermi level of electrons/holes. At the boundary of the active region, the Fermi level is pinned relative to the band edge due to the stimulated radiation. At the other boundary of the anode, as shown in Fig. S1 (also shown in Fig. 5 in the main text), \((E_c - E_{fn})\) reduces by 186meV when the injection level increases from the turn-on voltage (a) to 10kA/cm\(^2\) (b). As a result, the error \(e_c = 186\text{meV}\), introduced by replacing the Fermi level with the voltage drop (the drop of the band edge) is much smaller than the change of the Fermi level or the voltage drop \(U\) over the whole p area, which is about 1.75eV. This is due to a limited length of the p area, compared to the diffusion length of electrons [S1], as well as the exponential nature of the Boltzmann distribution. The former determines that the carrier concentrations do not change violently within a single layer due to recombination while the latter determines that the Fermi levels change gently with the carrier concentrations. The statement on the error \(e_p\) of the hole Fermi level is similar. This approximation is applied in Eq. (8) in the main text:

\[
\frac{dI_n}{dj} = \frac{d\Delta E_{fn}}{er_n} + \frac{d\Delta E_{fp}}{er_p} = \frac{dU + d\Delta e_p}{er_n} = \frac{dU}{er_n} + \frac{dU}{er_p} = \frac{U}{er_n} + \frac{U}{er_p} = \frac{r_p}{r_n + r_p}
\]

(S1)
This assumption is only valid when dealing with the drop on the whole p area. When considering only a part of the p area, such as the upper waveguide layer, the change of \((E_c - E_{fn})\) or \((E_{fp} - E_v)\) can be large at the boundaries (near the EBL) with an increasing current as shown in Fig. S1. This is due to an accumulation of electrons caused by the blocking effect of the EBL. In this case, it is inappropriate to replace the Fermi level drop with the voltage drop. It is necessary to describe the system by using quasi-Fermi level drops rather than the real voltage drop because the former includes both drift and diffusion effects. When using the latter, the drops of the electron and hole band edges are always the same within a single layer. The equivalent circuits of the theories using the Fermi level drop (a) and the real voltage drop (b) as the quasi voltage are different as shown in Fig. S2.

Fig. S2. The equivalent circuits of the p area of the LD when (a) Fermi-level drop and (b) real voltage drop are chosen as the quasi voltage drop.

2. The transmittance of the EBL

According to the thermal emission theory [S2], when the electrons flow to a heterojunction barrier,
only those with an energy higher than the barrier can cross. From the theory of semiconductors [S2], the electron concentration at the well side of the heterojunction is

\[ n_\text{c,w} = N_\text{c} \exp \left( - \frac{E_{\text{cw}} - E_{\text{fn}}}{k_B T} \right) \]

And by the thermal emission theory, the concentration at the barrier side is

\[ n_\text{c,b} = N_\text{c} \exp \left( - \frac{E_{\text{cb}} - E_{\text{fn}}}{k_B T} \right) \]

as if the Fermi level is the same as the well side [S3,S4], as illustrated in Fig. S3. Here \( N_\text{c} \) is the effective density of states and we have ignored the difference in it between the barrier and the well for simplicity. Hence, the transmittance of the electrons through an EBL with a conductive band difference \( \Delta E_c \) is:

\[ P_T = \frac{N_\text{c} \exp \left( - \frac{E_{\text{cb}} - E_{\text{fn}}}{k_B T} \right)}{N_\text{c} \exp \left( - \frac{E_{\text{cw}} - E_{\text{fn}}}{k_B T} \right)} = \exp \left( \frac{\Delta E_c}{k_B T} \right) \]

(S2)

Notice that a constant transmittance also guarantees a proportion between the electron concentrations of the waveguide layer and the cladding layer in the LED case, since in some cases there are also p-AlGaN layers in LEDs. Thus, in the LED case, our method of treating the electron resistance of the whole p area inversely proportional to the electron concentrations from the beginning of the p area is reasonable.

Fig. S3. Schematic diagram of electrons flowing over a heterojunction via the thermal emission mechanism. The electrons flow from the left to the right.

3. Drift-diffusion model in LDs

As is mentioned above, the low-energy electrons driven by the forward electric field in the upper waveguide layer will be blocked and bounced back by the EBL, gaining a reverse velocity against the electric field as illustrated in Fig. S4. Eventually, they will slow down and accumulate near the heterojunction and form a spatially descending concentration distribution, macroscopically causing a reverse diffusion current against the electric field and increasing the effective electron resistance of the waveguide layer. Let the coordinate origin be at the heterojunction between the waveguide layer and the EBL, \( x \) be the distance from the origin and the increasing direction be the direction of the current.
\( n(x) \), \( p(x) \) and \( E(x) \) are the electron concentration, hole concentration, and the electric field with coordinate respectively. The drift-diffusion equation is obtained [S2]:

\[
j_n = e\mu_n \left[ n(x)E(x) + \frac{k_B T}{e} \frac{dn}{dx} \right]
\]

(S3)

\[
j_p = e\mu_p \left[ p(x)E(x) - \frac{k_B T}{e} \frac{dp}{dx} \right]
\]

(S4)

To strictly solve the equations above, the Poisson equation and the charge-neutral condition \( n(x) = p(x) \) should be introduced and solved self-consistently. But here we only assume a constant electric field in a small range near the heterojunction:

\[
j_n = e\mu_n \left[ n(x)E + \frac{k_B T}{e} \frac{dn}{dx} \right]
\]

(S5)

At the heterojunction, electrons with a concentration of \( P_T n(0) \) will cross the EBL and contribute to a leakage current in the cladding layer:

\[
j_n = e\nu_e P_T n(0)
\]

(S6)

Notice that \( j_n \) must be equal everywhere in the whole p area to satisfy a current continuity when the recombination is negligible outside the active region. Thus, at a given \( j_n \), Eq. (S5) and (S6) are enough for a problem of boundary condition, whose solution is:

\[
n(x) = j_n \left( \frac{1}{e\nu_e P_T} - \frac{1}{e\mu_n E} \right) \exp \left( -\frac{eE}{k_B T} x \right) + \frac{j_n}{e\mu_n E}
\]

(S7)

The exponential behavior of Eq. (S7) explains the simulation results in Fig. 5(c) in the main text. The carrier concentration is proportional to the leakage current. Therefore, the reverse diffusion current is proportional to the leakage current assuming an exponential form of the electron distribution. Larger \( P_T \) will lead to a larger reverse diffusion current as well. The characteristic length \( \lambda = k_B T / eE \) of the electron gradient distribution in the waveguide layer is about 20nm with an electric field of \( 10^4 \) V/cm at a current density of 10kA/cm\(^2\).
4. Recombination in the upper waveguide layer

One of the possible problems of placing the EBL after the waveguide layer is that a relatively high concentration of electrons may recombine with holes in the waveguide layer. Fig. S5 Shows (a) the radiative recombination rate and (b) the electron current density of the p area of a typical LD structure in the main text at a current density of 20kA/cm². It is obvious that the recombination in the waveguide layer is negligible compared to that in the quantum well.

5. Energy levels in the quantum well

In the numerical simulation, the Poisson-Schrodinger equation is solved self-consistently for the quantum well. Fig. S6 shows a band diagram and the wave function of several sub-band energy levels in the quantum well near the turn-on voltage. Although there are two electron sub-bands in the quantum well, only the lower one dominates in luminescence due to the thermal distribution. The selection rule decides that the main inter-band transition occurs between the first conductive sub-band and the first...
valance sub-band. It is shown in Fig. S6 that at the turn-on voltage, $E_{fn} - E_{cw}$ is about a hundred meV and will be larger when the current increases, much larger than $k_B T = 26$ meV as is mentioned in the main text. Thus, we apply the approximation (also in the main text) since the exponential term is much larger than one:

$$n_w = g k_B T \ln \left[ 1 + \exp \left( \frac{E_{fn} - E_{cw}}{k_B T} \right) \right] \approx g \left( E_{fn} - E_{cw} \right)$$  \hspace{1cm} (S8)

Fig. S6. Energy levels and the wave functions in the quantum well.

Fig. S7 shows schematically how the electron concentration increases when the Fermi level is lifted at room temperature. When the Fermi level increases from 110 meV to 130 meV, the change of the average numbers of the state occupied by an electron is the area of the shade, which is approximately equivalent to the area of the rectangle enclosed by the dashed line:

$$\Delta n_w \approx g \Delta E_{fn}$$  \hspace{1cm} (S9)

The approximation is used in the main text.
6. Self-heating effect in the LEDs

To study the leakage current effect on the efficiency droop phenomenon of LEDs, the self-heating effect must be excluded. We apply up-to-500mA (2.5kA/cm$^2$) pulsed current with a 10$\mu$s pulse width and a 30Hz frequency on the LED sample and measure its luminescence intensity. As a reference, a continuous current is applied afterward. The duty ratios of the pulses are 0.03% and 100% respectively. The results are shown in Fig. S8. The results show no significant difference between the pulse condition and the continuous condition. Therefore, the self-heating effect in our experiments is negligible. This may be due to the small sizes of the LEDs.

![Fig. S8. The power-current curves of the LED under different pumping current conditions.](image)

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