Quantum model for carrier capture time through phonon emission in InGaN/GaN LEDs

Marco E. Vallone*, Francesco Bertazzi*†, Michele Goano*†, Giovanni Ghione*
* Dipartimento di Elettronica e Telecomunicazioni, Politecnico di Torino, corso Duca degli Abruzzi 24, 10129 Torino, Italy
† IEIIT-CNR, Politecnico di Torino, corso Duca degli Abruzzi 24, 10129 Torino, Italy
E-mail: marco.vallone@polito.it

***Abstract*—A quantum model is developed to obtain electron capture time in a quantum well through electron–longitudinal optic phonon emission, as function of carrier density, showing the interplay between phonon and collective plasma modes. We demonstrate that the usual approximation of a constant capture time in modeling of light-emitting diodes is not adequate, because this parameter varies considerably with the device working point.**

I. Introduction

Performance of InGaN/GaN light-emitting diodes (LEDs) depend critically on carrier transport across quantum wells (QWs) [1]. In particular, carrier capture time τ_c through longitudinal optic (LO) phonon emission and phonon-assisted Auger recombinations [2], [3] play an important role. We present a quantum model for the calculation of τ_c in InGaN/GaN QWs confirming the observed τ_c remarkable dependence on carrier density [4]. Our approach calculates τ_c from first principles as a function of temperature T, QW parameters and carrier density N_{B} in the bulk barrier states, evaluating self-consistently the carrier density N_{W} in the QW bound levels. As a result, we demonstrate the need to consider τ_c not as an external fitting parameter, but as a function of the LED working point and characteristics, in order to describe the underlying physics.

II. Model and method

Carriers are captured into QW from bulk barrier states in a time given by $1/\tau_c = 2/\hbar\Im(\Sigma_r)$, where $\Im(\Sigma_r)$ is the imaginary part of the retarded self-energy [5], [6]

$$\Sigma_r(\boldsymbol{k},\omega) = -(\beta\hbar)^{-1}\sum_{\boldsymbol{q},\omega_m} V_{\text{eff}}(\boldsymbol{q},\omega_m)\, G(\boldsymbol{k},\boldsymbol{q},\omega_m)\ . \quad (1)$$

Here $V_{\text{eff}}(\boldsymbol{q},\omega_m)$ is the density- and T-dependent screened potential interaction, G is the dressed propagator of a carrier of momentum $\hbar\boldsymbol{k}$ and energy $\hbar\omega$, whereas β and $\hbar$ are the inverse temperature in energy units and the reduced Planck's constant. As an example of this method, we addressed the Frölich interaction, describing the capture through emission of a LO-phonon-plasmon mode of energy $\hbar\omega_m$ and momentum $\hbar\boldsymbol{q}$, with $\boldsymbol{q} = (q, q_z)$. The imaginary part of the resulting self-energy Σ_r yields the capture time τ_c for this process and enters as well in the calculation of phonon-assisted Auger recombination coefficients [3]. In the end, τ_c can be employed in modeling tools as a function of LED working point (carrier density, temperature, etc.) and characteristics, and no more as a parameter. The interaction matrix element

$$V_{\text{eff}}(\boldsymbol{q},\omega_m) = -\int d\boldsymbol{r}\frac{1}{2\pi}\int dq_z \Psi^*_{\text{QW}}(\boldsymbol{r})\,\frac{4\pi e^2}{\epsilon_0\epsilon_s|\boldsymbol{q}|^2} \times \frac{D(|\boldsymbol{q}|,\omega_m)}{\epsilon^2(|\boldsymbol{q}|,\omega_m)}\Psi_{\text{bulk}}(\boldsymbol{r}) \quad (2)$$

depends on carrier density through the phonon dressed propagator $D(|\boldsymbol{q}|,\omega_m)$ and the dynamic dielectric function $\epsilon(|\boldsymbol{q}|,\omega_m)$, evaluated according to the Single Plasmon Pole (SPP) description of the Random Phase Approximation (RPA) [5], [6], whereas the QW and barrier wavefunctions Ψ_{QW} and Ψ_{bulk} determine the overlap integral. We obtained $\tau_c(N_B, N_{\mathrm{W}}, T)$ in a closed form, exploiting analytic integration in the ω_m and q complex plane, having extended to InGaN/GaN systems the approach fully described in [5] for III-V alloys.

III. Simulation results

To illustrate the method in practice, we considered for simplicity a $In_{0.85}Ga_{0.15}N$/GaN single QW system with flat bands. QW bands and electron and hole eigenfunction profiles have been evaluated in the effective mass approximation, obtaining strain-dependent energy gap and band offset according to [7]. For each value of QW width L_{W}, we calculated eigenvalues and eigenfunctions entering in (2) (an example is given in Fig. 1, for the conduction band). Self-energy Σ_r is evaluated versus N_{B} through (1) and (2), by means of which we obtain self-consistently N_{W} and τ_c for this scattering mechanism. Capture can take place through emission of any of two possible coupled phonon-plasmon modes of frequency ω_+, ω_-, with corresponding times τ_+, τ_- (as defined in [5]). In Fig. 2 capture times for electrons τ_+, τ_- are separately plotted for $L_{\mathrm{W}} = 3\,\mathrm{nm}$, and the resulting total $\tau_c = (1/\tau_+ + 1/\tau_-)^{-1}$ is shown in Fig. 3 as function of N_{B}, for three values of L_{W}. For the lowest carrier density values, τ_c results around 0.1 ps, but for an anti-screening effect [5] the capture time progressively reduces as N_{B} increases. However, when N_{B} exceeds $\approx 10^{18}\,\mathrm{cm}^{-3}$ the energy conservation prohibits the fastest of the two modes (ω_+), and capture can take place only through the slower mode (ω_-). We can appreciate one of the effects induced by the density dependent τ_c looking at carrier density N_{W} on the QW bound level versus N_{B},

978-1-4799-3682-3/14/$31.00 ©2014 IEEE

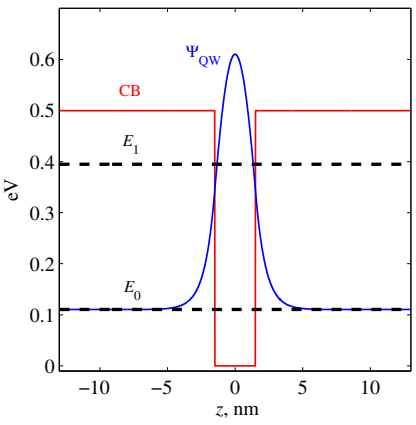

Fig. 1. Conduction band (CB) energy profile, for L_W = 3 nm, with two confined levels $E_{0,1}$. The ground-state eigenfunction Ψ_{QW} is also shown.

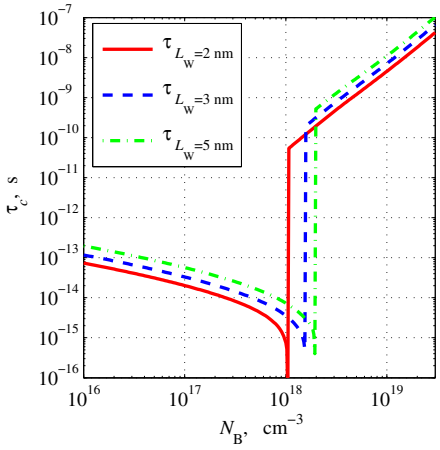

Fig. 3. Total electron capture times for LO-phonon emission, for three QW width values (L_W = 2, 3, 5 nm).

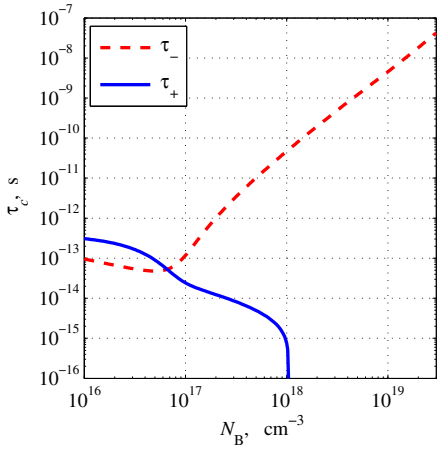

Fig. 2. Electron capture times through the phononic modes ω_+, ω_- for L_W = 3 nm.

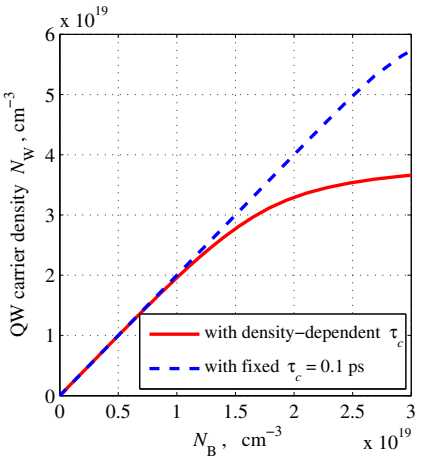

Fig. 4. Carrier density N_W on the QW bound level versus barrier states carrier density N_B, for L_W = 3 nm.

shown in Fig. 4, obtained self-consistently, considering a two-populations LED rate equation system for N_B and N_W in stationary regime. The effect of the great increase of τ_c with N_B is well evident (solid line), in comparison with employing a constant τ_c (dashed line).

IV. Conclusion

All these facts indicate a capture time and self-energy that are extremely variable with carrier density. This quantum model allows to semi-analytically calculate $\Im(\Sigma_r)$ and τ_c, abandoning – when possible – the too simple approach of a single-value approximation (e.g. the often used $\tau_c \approx 0.1$ ps) in LED simulations. We stress that this work is only an example of a methodology applicable to all other phonon modes and carrier-carrier scattering. Furthermore it can be easily extended to more realistic QW models, without substantial modifications. Capture time, when polarization charges warp eigenfunctions, scales to significantly longer values, but the overall behavior with density is maintained.

References

[1] G. Verzellesi, D. Saguatti, M. Meneghini, F. Bertazzi, M. Goano, G. Meneghesso, and E. Zanoni, "Efficiency droop in InGaN/GaN blue light-emitting diodes: Physical mechanisms and remedies," *J. Appl. Phys.*, vol. 114, no. 7, p. 071101, Aug. 2013.

[2] E. Kioupakis, P. Rinke, K. T. Delaney, and C. G. Van de Walle, "Indirect Auger recombination as a cause of efficiency droop in nitride light-emitting diodes," *Appl. Phys. Lett.*, vol. 98, no. 16, p. 161107, 2011.

[3] F. Bertazzi, M. Goano, and E. Bellotti, "Numerical analysis of indirect Auger transitions in InGaN," *Appl. Phys. Lett.*, vol. 101, no. 1, p. 011111, July 2012.

[4] W. H. Fan, S. M. Olaizola, J.-P. R. Wells, A. M. Fox, T. Wang, P. J. Parbrook, D. J. Mowbray, and M. S. Skolnick, "Femtosecond studies of electron capture times in InGaN/GaN multiple quantum wells," *Appl. Phys. Lett.*, vol. 84, no. 16, pp. 3052–3054, Apr. 2004.

[5] M. E. Vallone, "Quantum well electron scattering rates through longitudinal optic-phonon dynamical screened interaction: An analytic approach," *J. Appl. Phys.*, vol. 114, no. 5, p. 053704, Aug. 2013.

[6] G. D. Mahan, *Many-Particle Physics*, 2nd ed. New York: Plenum Press, 1990.

[7] S. Chiaria, E. Furno, M. Goano, and E. Bellotti, "Design criteria for near-ultraviolet GaN-based light-emitting diodes," *IEEE Trans. Electron Devices*, vol. 57, no. 1, pp. 60–70, Jan. 2010.