Auger transitions and their signatures in III-nitride LEDs: a full-band modeling

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***Abstract*—Auger recombination and the relaxation of the resulting excited electrons are investigated in III-nitride light-emitting diodes (LEDs) with a full-band Monte Carlo carrier transport model to assess the possibility of recovering Auger signatures from experiments. Full-Brillouin-zone calculations of Auger coefficients indicate that Auger recombination may not be negligible for LED operation, although the identification of Auger signatures from complex experiments should be supported by theoretical calculations before any claim concerning the origin of the efficiency droop can be made.**

Auger processes are at the heart of the debate concerning droop, the decline of the internal quantum efficiency in nitride-based light-emitting diodes (LEDs) at high injection currents. [1] Most experimental investigations dealing with Auger losses in GaN-based light-emitters have attempted to estimate loss coefficients with simple power laws. Originally, Auger losses were blamed for droop on account of their dependence on the excitation density which seemed to match experimental ABC efficiency data. Recently, two notable experiments [2], [3] have reported the direct observation of hot carriers excited by Auger recombination in the active region of GaN-based light emitters.

Iveland et al. studied the energy distribution curves (EDCs) of the electrons emitted from the cesiated GaN p-cap (the highly Mg-doped layer between the active region and the anode contact) of a forward-biased InGaN/GaN LED. [2] At least two distinct peaks were observed in the EDCs. The lower-energy peak was attributed to photoemitted electrons excited in the band bending region (BBR, near the surface of the GaN p-cap) by the light generated in the active region. The higher-energy peak was ascribed to the presence, at the p-cap surface, of a population thermalized at the bottom of an upper valley of the conduction band (CB) of GaN, derived from high-energy electrons excited by Auger recombination processes in the active region.

Binder et al. optically pumped into droop regime a test structure composed of alternating ultraviolet (UV) and green quantum wells (QWs) using a high-power laser source at a wavelength that is resonant with the green QWs, but energetically below the UV ones. [3] For test devices that contained only UV QWs, no UV photoluminescence was detected. However, in the devices with both kinds of wells, emission from the UV QWs was observed in addition to that of the green ones. The observed UV luminescence was ascribed to hot electrons escaping the green QWs by Auger transitions and subsequently captured by the UV QWs, loss channels caused by carrier transport issues being ruled out by the optical injection.

The interpretation of both experiments is still under debate. On the one hand, many-body calculations [4] performed by Hader et al. indicate that Auger processes are not necessary to explain the photoluminescence spectra observed in Ref. [3]. In fact, while the excitation pulse itself is spectrally narrow, the polarization excited in the material dephases on a very fast timescale due to carrier-carrier and carrier-phonon scattering processes. Thus luminescence from the UV wells cannot be unequivocally interpreted as the signature of Auger processes, but may be ascribed to the dephasing of the induced microscopic polarization which generates carriers directly in the UV wells.

On the other hand, a full-band Monte Carlo carrier transport analysis [5] suggests that the interpretation of Ref. [2] is not plausible. A critical assumption in Ref. [2] is that Auger electrons collected in the satellite *L valley* would not undergo significant relaxation towards Γ_1^c before reaching the BBR. In particular, it was argued that high-energy Auger electrons, would quickly thermalize in the *L valley*, and cross the 200 nm-thick highly-doped GaN p-cap (plus a 40 nm-thick electron blocking layer) with a transit time estimated at 1 ps, corresponding to a velocity of 2×10^7 cm/s. [2] But, this velocity implies ballistic transport, which undermines the claim that *thermalized* electrons populate the satellite valley. Another questionable assumption is that the electrons would be trapped in the long-lived upper valleys with a scattering time to the bottom of he Γ valley of about 1 ps. [2] As diffusion is the only viable transport mechanism in a region where the electric field is negligible, in order to have a sizable fraction of carriers surviving after 240 nm in the L valley, one should assume a scattering time from L to Γ_1^c in excess of 100 ps, which is in stark contrast with intervalley deformation potential scattering rates computed e.g. by Goodnick *et al.* [6] and by our group. [7] In addition to deformation potential scattering, polar optical emission is also a very efficient relaxation mechanism in GaN,

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since the LO phonon energy is 90 meV and the coupling is stronger by one order of magnitude compared to other polar III-V materials. The interpretation of the observed emission spectra are also not compatible with the electronic structure of GaN. In particular, the position of the high-energy peak shifts with bias, an effect possibly related to the rectifying behavior of the cesiated contact. [2] According to Ref. [2], the vacuum level is 2.3 eV above the Fermi level, and 2.5 eV above the bulk p-type valence band. At 4 mA, the higher-energy peak is located at 1.5 eV above the vacuum level, i.e. just 0.5 eV above the bulk conduction band edge. Therefore, the position of the high-energy emission peak is at odds with all modern DFT electronic structure calculations, which place satellite valleys in GaN above 2 eV. [8], [9]

Having discussed merits and potential pitfalls of recent experimental efforts to recover Auger signatures in GaN-based LEDs, we now turn our attention to theoretical investigations of Auger transitions in III-nitrides. It is now accepted that direct Auger recombination is negligible in bulk InGaN [10] as well as in comparable wide band gap material systems. [11] This result is in agreement with the expectation that Auger recombination in wide-gap semiconductors is dominated by indirect (i.e. phonon-assisted) transitions, due to the large threshold resulting from energy and momentum conservation. Indirect Auger processes in bulk InGaN were studied with *ab initio* approaches, leading to Auger coefficients $C_{3D} \approx 3\times10^{-31}\,\mathrm{cm^6 s^{-1}}$ in Ref. [12]. Similar calculations performed within a Green function technique predicted lower values and a stronger dependence on the energy gap [13]. Both Refs. [12], [13] neglected quantizations effects. Microscopic theories of Auger recombination in QWs, [14] relying on multiband $\boldsymbol{k}\cdot\boldsymbol{p}$ models within the envelope-function approximation (EFA) predicted a significant enhancement of Auger rates due to the lack of momentum conservation along the confining direction. Although successful for zincblende quantum systems, the application of EFA theories to GaN-based QWs led to discordant results. [15–17] Vaxenburg et al. argued that sharp interfaces of the wells lead to high momentum contributions to the wavefunctions resulting in Auger coefficients high enough to explain droop. However, the dependence on the confinement potential was also investigated in Ref. [15] by comparing results for quantum wells with step-like interfaces to those for wells with Gaussian broadened potential; no strong influence of the details of the potential was found in Ref. [15]. These discrepancies may, at least in part, be explained by possible inconsistencies and intrinsic limitations of the underlying $\boldsymbol{k}\cdot\boldsymbol{p}$ model of the subband structure, since Auger transitions in wide gap materials involve both confined states near the band edges and excited states that lie far above the gap. FBZ calculations based on the model described in Ref. [18], indicate that direct Auger transitions in confined InGaN/GaN structures are (i) enhanced by the lack of momentum conservation along the confining direction (ii) have a strong variation with the well thickness with peak values comparable with bulk phonon-assisted processes and (iii) increase, although not dramatically, with the polarization fields, as a result of the increased spectral content of the confining potential. Detailed calculations of both eeh and hhe processes will be presented at the time of the presentation.

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] J. Iveland, L. Martinelli, J. Peretti, J. S. Speck, and C. Weisbuch, "Direct measurement of Auger electrons emitted from a semiconductor light-emitting diode under electrical injection: Identification of the dominant mechanism for efficiency droop," *Phys. Rev. Lett.*, vol. 110, p. 177406, Apr. 2013.

[3] M. Binder, A. Nirschl, R. Zeisel, Hager, H.-J. Lugauer, M. Sabathil, D. Bougeard, J. Wagner, and B. Galler, "Identification of nnp and npp Auger recombination as significant contributor to the efficiency droop in (GaIn)N quantum wells by visualization of hot carriers in photoluminescence," *Appl. Phys. Lett.*, vol. 103, no. 7, p. 071108, Aug. 2013.

[4] J. Hader, J. V. Moloney, and S. W. Koch, "Microscopic many-body investigation of the efficiency droop in GaN based light emitting devices," in *SPIE Photonics West, Gallium Nitride Materials and Devices VIII*, vol. 9003, Proceedings of the SPIE, San Francisco, CA, Feb. 2014, pp. 900 311–1–900 311–6.

[5] F. Bertazzi, M. Goano, X. Zhou, M. Calciati, G. Ghione, M. Matsubara, and E. Bellotti, "Comment on "Direct measurement of Auger electrons emitted from a semiconductor light-emitting diode under electrical injection: Identification of the dominant mechanism for efficiency droop" [Phys. Rev. Lett. 110, 177406 (2013)]," http://arxiv.org/abs/1305.2512, 2013.

[6] S. Yamakawa, S. Aboud, M. Saraniti, and S. M. Goodnick, "Influence of the electron-phonon interaction on electron transport in wurtzite GaN," *Semiconductor Sci. Tech.*, vol. 19, no. 4, pp. 475–477, Apr. 2004.

[7] F. Bertazzi, M. Moresco, and E. Bellotti, "Theory of high field carrier transport and impact ionization in wurtzite GaN. Part I: A full band Monte Carlo model," *J. Appl. Phys.*, vol. 106, no. 6, p. 063718, Sep. 2009.

[8] A. Svane, N. E. Christensen, I. Gorczyca, M. van Schilfgaarde, A. N. Chantis, and T. Kotani, "Quasiparticle self-consistent GW theory of III-V nitride semiconductors: Bands, gap bowing, and effective masses," *Phys. Rev. B*, vol. 82, p. 115102, Sep. 2010.

[9] L. C. de Carvalho, A. Schleife, and F. Bechstedt, "Influence of exchange and correlation on structural and electronic properties of AlN, GaN, and InN polytypes," *Phys. Rev. B*, vol. 84, p. 195105, Nov. 2011.

[10] F. Bertazzi, M. Goano, and E. Bellotti, "A numerical study of Auger recombination in bulk InGaN," *Appl. Phys. Lett.*, vol. 97, no. 23, p. 231118, Dec. 2010.

[11] M. Heinemann and C. Heiliger, "Auger recombination rates in ZnMgO from first principles," *J. Appl. Phys.*, vol. 110, no. 8, p. 083103, 2011.

[12] 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.

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

[14] J. Hader, J. V. Moloney, and S. W. Koch, "Microscopic evaluation of spontaneous emission- and Auger-processes in semiconductor lasers," *IEEE J. Quantum Electron.*, vol. 41, no. 10, pp. 1217–1226, Oct. 2005.

[15] J. Hader, J. V. Moloney, B. Pasenow, S. W. Koch, M. Sabathil, N. Linder, and S. Lutgen, "On the importance of radiative and Auger losses in GaN-based quantum wells," *Appl. Phys. Lett.*, vol. 92, no. 26, p. 261103, 2008.

[16] R. Vaxenburg, E. Lifshitz, and A. L. Efros, "Suppression of Auger-stimulated efficiency droop in nitride-based light emitting diodes," *Appl. Phys. Lett.*, vol. 102, no. 3, p. 031120, 2013.

[17] R. Vaxenburg, A. Rodina, E. Lifshitz, and A. L. Efros, "The role of polarization fields in Auger-induced efficiency droop in nitride-based light-emitting diodes," *Appl. Phys. Lett.*, vol. 103, no. 22, p. 221111, 2013.

[18] F. Bertazzi, X. Zhou, M. Goano, G. Ghione, and E. Bellotti, "Auger recombination in InGaN/GaN quantum wells. A full-Brillouin-zone study," *Appl. Phys. Lett.*, vol. 103, no. 8, p. 081106, Aug. 2013.