Title	Investigating the competition of radiative and nonradiative recombination in (In,Ga)N quantum wells
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Publication date	2023-10-09
Original Citation	Schulz, S., McMahon, J., Kioupakis, E., Barrett, R. M., Ahumada-Lazo, R., Alanis, J. A., Parkinson, P., Kappers, M. J., Oliver, R. A. and Binks, D. (2023) 'Investigating the competition of radiative and nonradiative recombination in (In,Ga)N quantum wells', 2023 International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD), Turin, Italy, 18-21 November, pp. 57-58. doi: 10.1109/NUSOD59562.2023.10273496
Type of publication	Conference item
Link to publisher's version	10.1109/nusod59562.2023.10273496
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Download date	2025-05-20 05:39:06
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Investigating the competition of radiative and nonradiative recombination in (In,Ga)N quantum wells

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***Abstract*—We present a combined theoretical and experimental analysis of Auger recombination in c-plane (In,Ga)N quantum wells. On the theoretical side we use an atomistic model that accounts for random alloy fluctuations to investigate the impact that temperature and carrier density has on the radiative and Auger recombination rate. Our calculations indicate a weak temperature dependence of the Auger rate compared to the temperature dependence of the radiative rate. However, with increasing carrier density the Auger rate increases more strongly when compared to the radiative rate. Our theory results indicate an onset of the efficiency drop at carrier densities $\gtrsim 1\times10^{19}$cm^{-3}, in very good agreement with our photoluminescence studies on similar (In,Ga)N quantum well samples. Overall, we find that alloy enhanced Auger recombination is sufficient to explain the experimental data investigated here.**

***Index Terms*—InGaN, quantum wells, carrier localization, Auger recombination**

I. INTRODUCTION

c-plane (In,Ga)N quantum wells (QWs) form the backbone of many modern violet/blue spectral range light-emitting diodes (LEDs). However, the efficiency of these devices has been observed to deteriorate as a function of temperature and carrier density. The reduction in efficiency that occurs as the device operating temperature increases is known as "thermal droop" [1], and the corresponding reduction with increasing carrier density is known as "efficiency droop" [2]. Auger recombination is a nonradiative three-carrier process which could facilitate these efficiency droops [2], however, the related competition between radiative and Auger recombination is still under debate. The theoretical modelling of Auger recombination is, in general, challenging, but is further complicated by alloy-fluctuation-induced carrier localization effects in (In,Ga)N systems. As such, fully three-dimensional simulations are required, which, in the case of an (In,Ga)N *QW*, lead to very large supercells. Due to the large number of atoms involved, standard density-functional theory (DFT) cannot be used to gain insight into the impact of alloy fluctuations on the Auger rate in (In,Ga)N QWs. Thus, semi-empirical models are required to address this question. Here, we employ an empirical atomistic tight-binding (TB) model that accounts for alloy fluctuation induced carrier localization effects, to calculate the temperature and carrier density dependence of the Auger rate in c-plane (In,Ga)N QWs. The model has been previously benchmarked against experimental and DFT data, and was recently used to gain insight into the temperature dependence of the radiative recombination rate [3]. Our calculations reveal that for a fixed carrier density the Auger rate only shows a weak temperature dependence (compared to the temperature dependence of the radiative recombination rate) indicating that factors other than Auger recombination (e.g. carrier escape) are more likely the origin of the thermal droop. The atomistic model is then used to evaluate the radiative and Auger rates over a wide range of carrier densities and to gain insight into the internal quantum efficiency (IQE); the obatined IQE is compared to experiment. The model demonstrates that whilst nonradiative recombination such as Shockley Read Hall (SRH) affects the peak IQE value and the carrier density corresponding to the onset of droop, for carrier densities $\gtrsim 1\times10^{19}$ cm^{-3} it becomes insignificant and IQE depends on the competition between radiative and alloy-enhanced Auger recombination, without any defect assistance.

II. THEORY AND EXPERIMENT

Here we briefly summarise the theoretical framework used to calculate the electronic structure, radiative and Auger recombination rates (including Auger coefficients) in c-plane (In,Ga)N/GaN QWs. Further details can be found in [3] and [4]. We investigate the electronic structure of a c-plane (In,Ga)N/GaN QW of width 3 nm, by means of an atomistic, nearest neighbor sp^3 tight-binding (TB) model. The indium content in the well is defined to be 15%. The well is embedded in GaN barriers and a supercell with periodic boundary conditions (approx. 82,000 atoms) is used. To analyze the impact of the alloy microstructure on the results, the calculations have been repeated several times with different random alloy configurations. A valence force field model is employed to determine the relaxed atomic positions. The obtained positions form input for a local polarization theory to determine the electrostatic built-in field characteristics for these c-plane (In,Ga)N QWs. The data are then connected to the TB model, which allows us to study the impact of alloy fluctuations on a microscopic level. The TB model employed here has been benchmarked and parameterized against DFT calculations and experimental studies. We note that the model accurately determines electronic states at higher (lower) lying energies, away from the conduction (valence) band edges, which are particularly important for the calculation of Auger coefficients. In order to account for the screening of the electrostatic built-in fields with increasing carrier density, we use the approach discussed in [5]. Equipped with the electronic structure model, we evaluate the radiative and Auger recombination rates by applying Fermi's Golden Rule [6]; required ingredients (wave functions, screened Coulomb matrix elements etc.) are directly calculated from the TB wave functions, thus including alloy fluctuations and their connected carrier localization effects. Once radiative and Auger rates are determined, the radiative (B) and Auger coefficients (C) are calculated as a function of temperature and carrier density. The ABC model [2] is used to obtain IQE values with SRH coefficients from literature [7].

On the experimental side, three samples were studied, each grown by metal organic chemical vapour deposition, and differing only in growth temperature of the well, which is intended to vary the point defect density, and hence nonradiative recombination rate. The experimental IQE values were determined by measuring the optical emission under resonant ultrafast pulsed laser excitation at room temperature.

III. RESULTS AND DISCUSSION

When studying the Auger recombination process as a function of the temperature but at a fixed carrier density ($n \approx 4 \times 10^{18}$ cm^{-3}), we find only a weak temperature dependence of the Auger rate. As discussed in [4], when analyzing this effect in conjunction with the temperature dependence of the radiative rate, we conclude that the here considered Auger process is of secondary importance to the thermal droop. Turning to the carrier density dependence of radiative and Auger rates, we observe that while the onset of the droop effect is affected by the choice of the A coefficient, for carrier densities beyond 1×10^{19}cm^{-3} the value of A is of secondary importance and the IQE depends mainly on the competition between radiative and alloy-enhanced Auger recombination as indicated in Fig. 1. We find that this observed behavior is in excellent agreement with our experimental data [7].

IV. SUMMARY AND OUTLOOK

Based on an atomistic electronic structure model that accounts for alloy fluctuation induced carrier localization effects, we have analyzed the temperature and carrier density dependence of Auger recombination in a c-plane (In,Ga)N/GaN QW. Our results support the conclusion that Auger recombination is not the driver behind the thermal droop in (In,Ga)N-based LEDs. Moreover, our combined theory-experiment comparison reveals that when using our localisation-enhanced radiative and Auger rates, the corresponding carrier density dependent IQE is in excellent agreement with our experimental measurements. In addition, our studies suggest that nonradiative processes external to the QWs, such as SRH and defect-assisted Auger recombination in the *barriers*, rather than Auger processes in the well, may contribute appreciably to low external quantum efficiencies of green LEDs.

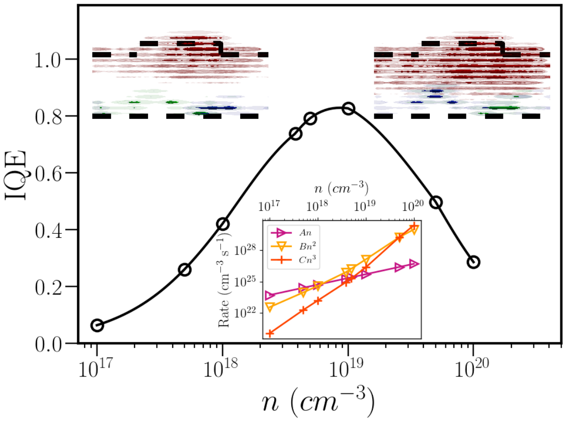

Fig. 1. Internal quantum efficiency of an In$_{0.15}$Ga$_{0.85}$N QW. The inset shows recombination rates for Shockley-Read-Hall (A), radiative (B) and Auger (C) processes. Example electron (red) and hole (blue: ground state; green: first excited state) charge densities in the QW are also given (left: carrier density $< 1 \times 10^{19}$ cm^{-3}, right: carrier density $> 1 \times 10^{19}$ cm^{-3}).

ACKNOWLEDGMENTS

The authors acknowledge the financial support by SFI (Grant Nos. 17/CDA/4789 and 12/RC/2276 P2), the University of Michigan Blue Sky Research Program, EPSRC (Grant Nos. EP/M010589/1 and EP/M010627/1, and Doctoral Training Partnership studentships), and UKRI for a Future Leaders Fellowship (MR/T021519/1). Computing resources provided by the SFI and Higher Education Authority (HEA) funded Irish Centre for High End Computing are acknowledged.

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