Theoretical Study of the Temperature Dependent Competition of Non-radiative Auger-Meitner and Radiative Recombination in (Al,Ga)N Quantum Wells

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Light emitting diodes (LEDs) operating in the (deep) ultraviolet (UV) spectral region that utilize the wide band gap semiconductor alloy aluminium gallium nitride, (Al,Ga)N, have attracted significant interest in recent years. When compared to conventional mercury-based UV emitters, (Al,Ga)N LEDs offer, in principle, light emitters that are more energy efficient, wavelength tuneable and more environmentally friendly. However, in comparison to other III-N LEDs, such as those based on (In,Ga)N alloys operating in the visible wavelength range, deep UV (Al,Ga)N LEDs exhibit in general (very) low external quantum efficiencies [1]. A variety of different factors have been highlighted in the literature that contribute to this disparity in the efficiency of visible and UV LEDs [1]. Overall, we note that the fundamental properties of (Al,Ga)N-based quantum wells (QWs) lying at the heart of these LEDs are not well understood. Moreover, in general, III-N heterostructures exhibit very different properties compared to their III-As counterparts, including, for instance, that random alloy fluctuations are sufficient to lead to strong carrier localization. Such effects are often neglected in theoretical studies of (Al,Ga)N QW systems.

In this work we study the electronic structure, radiative and non-radiative recombination processes in an $Al_{0.5}Ga_{0.5}N$/AlN QW system. To gain insight into the electronic properties of the wells, we employ an atomistic empirical tight-binding model that is coupled to a valence force field and a local polarization field model [2]. In doing so, the local strain and polarization fields can be described on a microscopic level. Given the atomistic nature of our electronic structure theory, information about the alloy microstructure is required as input to our studies. In line with experimental investigations, we consider random alloy fluctuations in the $Al_{0.5}Ga_{0.5}N$ QW, which reflects the situation observed in (In,Ga)N QW systems [3,4]. Our calculations reveal that, similar to (In,Ga)N wells, random alloy fluctuations are already sufficient to lead to carrier localization effects [2].

Equipped with the electronic structure, we evaluate non-radiative Auger-Meitner recombination as well as radiative recombination rates and their connected C and B coefficients, respectively, as a function of temperature, as we have previously done for (In,Ga)N QWs [5]. The temperature dependent competition of these rates may then provide insight into the so-called thermal "droop" observed in (Al,Ga)N-based LEDs [6]. At a fixed carrier density of $n=2.5\text{x}10^{18}$ cm^{-3} and a well width of 2.85 nm, our calculations reveal Auger-Meitner coefficients in the range of $C=5\text{x}10^{-32}$ cm^6 s^{-1} to $C=1\text{x}10^{-31}$ cm^6 s^{-1}, and radiative coefficients in the range of $B=2\text{x}10^{-13}$ cm^3 s^{-1} to $B=5\text{x}10^{-13}$ cm^3 s^{-1}. Moreover, for the carrier density considered here, our studies show a weak temperature dependence of the B coefficient, while the C coefficient decreases with increasing temperature. Thus, our calculations indicate that non-radiative Auger-Meitner recombination may not be a significant contributor to the *thermal droop* in (Al,Ga)N QW-based UV emitters and so other factors, such as carrier injection or defect-related processes, may play a more prominent role.

References

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