Theoretical investigation of carrier transport and recombination processes for deep UV (Al,Ga)N light emitters

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***Abstract*—We present a theoretical study on the impact of alloy disorder on carrier transport and recombination rates in an (Al,Ga)N single quantum well based LED operating in the deep UV spectral range. Our calculations indicate that alloy fluctuations enable 'percolative pathways' which can result in improved carrier injection into the well, but may also increase carrier leakage from the well. Additionally, we find that alloy disorder induces carrier localization effects, a feature particularly noticeable for the holes. These localization effects can lead to locally increased carrier densities when compared to a virtual crystal approximation which neglects alloy disorder. We observe that both radiative and non-radiative recombination rates are increased. Our calculations also indicate that Auger-Meitner recombination increases faster than the radiative rate, based on a comparison with a virtual crystal approximation.**

I. Introduction

The past few decades have shown a strong need for developing efficient and wavelength tuneable ultraviolet (UV) light emitters, given their potential and importance for a wide range of applications across the entire UV spectrum [1]. One region of particular interest is the deep UV range ($<$ 280 nm) for use in e.g., water purification, medical sterilization, sensing etc. [1]. The direct band gap semiconductor aluminium gallium nitride ((Al,Ga)N) is in principle an ideal candidate for developing light emitting diodes (LEDs) addressing the entire UV spectral window. However, current state-of-the-art UV light emitting devices exhibit very low efficiencies [1]. In the deep UV range this problem is particularly pronounced with multiple factors contributing to this effect. In order to overcome these very low efficiencies, understanding the fundamental properties of (Al,Ga)N-based heterostructures and how these properties affect the device performance is of central importance. Here, simulation studies can contribute to identifying these key factors and ultimately help to design more efficient devices.

However, recent studies have highlighted that the theoretical description of nitride-based light emitters presents significant challenges when compared to other conventional III-V semiconductor systems [2]. It has been shown that alloy disorder can induce carrier localization effects, which play a crucial role for understanding electronic, optical and transport properties of, for instance, indium gallium nitride (InGaN) based light emitters. Most commercially available software packages do not account for such effects. Moreover, in comparison to (In,Ga)N-based systems, the understanding of the impact of alloy disorder on carrier transport and also carrier recombination processes is sparse for (Al,Ga)N systems. However, recent experiments [3] and simulations [4] indicate that (Al,Ga)N quantum wells (QWs) also exhibit carrier localization effects due to random alloy fluctuations. In this work, building on a multiscale simulation framework, we address the influence of random alloy fluctuations on carrier transport and the competition between radiative and non-radiative (Auger-Meitner) recombination in an (Al,Ga)N based LED.

II. Method

Our multiscale simulation framework connects a three-dimensional (3D) atomistic semi-empirical tight binding model, that accounts for alloy and connected fluctuations in strain and built-in fields on a microscopic level [4], to a macroscopic drift-diffusion model [5,6]. Quantum corrections are included here via localization landscape theory [7].
The model is applied to a 2.3 nm wide *c*-plane $Al_{0.7}Ga_{0.3}N$ single QW with $\approx$10 nm intrinsic $Al_{0.8}Ga_{0.2}N$ barriers embedded in a p-n junction with doping densities of 5×10^{19} cm^{-3}. To investigate the impact of alloy fluctuations on carrier transport and recombination processes, the results of our atomistic studies are compared to the outcome of calculations in which the intrinsic region (QW and barriers) is treated as a homogenous alloy that can be described by averaged material parameters. The latter approximation is often called a virtual crystal approximation (VCA) and is widely employed in commercially available software packages.

III. Results

Employing the full 3D atomistic description of the (Al,Ga)N device, we find that the presence of random alloy disorder

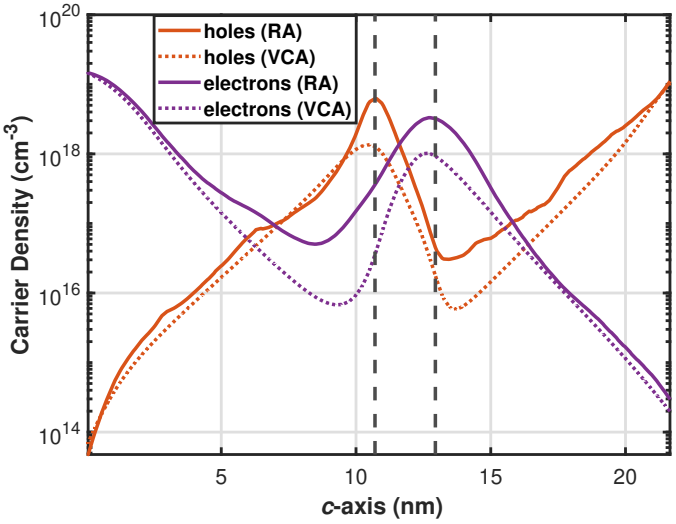

Fig. 1. Log plot of electron (purple) and hole (orange) densities along the c-axis of the 3D $Al_{0.7}Ga_{0.3}N/Al_{0.8}Ga_{0.2}N$ quantum well and intrinsic barriers at $\approx$ 5.4 V for both the random alloy (RA) system and virtual crystal approximation (VCA). The random alloy results have been averaged at each plane along the c-axis. The black dashed lines indicate the quantum well boundaries.

leads to large variations in both conduction and valence band edge energies of the intrinsic active region (QW and intrinsic barriers). These alloy induced fluctuations in the band edge energies can open up 'percolative pathways', regions of lower band gaps which form a preferential path for the current to follow. This allows for an enhanced carrier injection into the QW when compared to a VCA treatment, which is intrinsically not capturing these lower band gap regions. A consequence of an improved carrier injection into the QW is then reflected in a higher carrier density in the QW at a fixed bias. Figure 1 gives an example of the differences in carrier densities extracted from our atomistic treatment and the VCA description. However, Fig. 1 also reveals an increase in the carrier densities in the (Al,Ga)N barrier due to alloy disorder. This finding suggests that percolative pathways, in addition to promoting carrier injection into the QW, may also lead to increased carrier leakage from the QW. While at first glance this may be regarded as a detrimental effect, it may be used to tailor and improve inter-well transport in multi-QW systems to achieve a more evenly distributed carrier density.

While Figure 1 shows the carrier density averaged over each c-plane in the system, our atomistic calculation also reveals that locally the carrier densities can strongly exceed the average value, in particular for holes. This effect is attributed to alloy induced carrier localization effects. We find that a consequence of this is an increase in both the radiative and non-radiative Auger-Meitner recombination rates for the random alloy system when compared to the VCA description. This increase in the Auger-Meitner recombination and the increase in the resulting high energy carriers may lead to generating defects in (Al,Ga)N based UV emitters, as recent experimental studies indicate [8].

IV. Conclusion

In conclusion, our multi-scale simulations of the carrier transport and recombination processes in a 3D c-plane deep UV single (Al,Ga)N QW LED indicate that alloy disorder may lead to (i) an enhancement in the carrier injection into the QW at lower bias values, when compared to a VCA description, due to the presence of 'percolative pathways', (ii) an increase in carrier leakage from the well again facilitated by percolative pathways and (iii) an increase of local carrier densities due to alloy induced carrier localization effects. The latter aspect can lead to increased radiative, but also non-raditive Auger-Meitner recombination processes, which can have a detrimental impact on the device performance. Therefore, our calculations already indicate that a careful design of the active region (e.g. by using a multi-QW system to reduce, and ideally evenly distribute, the carrier density between the wells) is required. To guide the design of such a structure from a theoretical perspective, the above discussed factors have to be considered in realistic simulations. The here established methods and models are now an ideal starting point for such a task.

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