Theoretical investigation of optical polarisation in alloy disordered (Al,Ga)N quantum well systems

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***Abstract*—Aluminium Gallium Nitride ((Al,Ga)N) is an ideal material for light emitting devices in the UV spectral range. However, these devices still suffer from low external quantum efficiencies, particularly in the deep-UV range. A contributor to the low external quantum efficiency is low light extraction efficiency (LEE), which is tightly linked to the valence band structure of (Al,Ga)N quantum wells. Theoretical studies that account for alloy disorder-induced valence band mixing effects in these structures are sparse. Here, we utilise an atomistic multi-band tight-binding model to gain insight into the degree of optical polarisation in (Al,Ga)N quantum well systems. Special attention is paid to the impact of Al content, well width and carrier density in the wells.**

***Index Terms*—UV-C emitters, alloy disorder, light polarization, Urbach tail energies**

I. Introduction

Thanks to their large direct band gap, Aluminium Gallium Nitride ((Al,Ga)N) alloys have attracted significant attention for UV light-emitting applications [1]. A region of particular interest is the UV-C wavelengths window ($<$ 280 nm), which can be used for applications such as water purification, sterilization, etc. [1]. However, (Al,Ga)N-based light emitting diodes (LEDs) suffer from low quantum efficiencies at wavelengths in the UV-C range, stemming in part from a low light extraction efficiency (LEE) [1]. The overall low LEE is related to differences in the valence band structure of AlN and GaN and how the band character changes with Al content in (Al,Ga)N heterostructures such as quantum wells (QWs). Here, the crystal field splitting energy, Δ_{cf}, plays an important role. For GaN, Δ_{cf} is positive ($\approx +30$ meV), while in AlN Δ_{cf} is *negative* (≈ -200 meV) [2]. As a result, the valence band edge (VBE) of GaN has Γ_9 symmetry, which is made up of p_x, p_y like orbitals, whereas the VBE in AlN is of Γ_7 symmetry, composed of mainly p_z like orbitals. The symmetry of the highest valence states for GaN and AlN gives rise to the emission of transverse electric (TE) and transverse magnetic (TM) polarized photons, respectively [3]. Given that standard LEDs are surface emitting devices, TM polarised light leads to a very low LEE.

This work received funding from the Leibniz Competition 2022 (UVSimTec, K415/2021), the Sustainable Energy Authority of Ireland and Taighde Éireann – Research Ireland (17/CDA/4789, 12/RC/2276 P2 and 21/FFP-A/9014), and the Leibniz competition 2020 (NUMSEMIC, J89/2019).

The relative emission of TM and TE polarized light can be described by the degree of optical polarisation (DOP), which depends on the orbital character of the valence states contributing to the light emission process. In addition to heterostructure confinement, strain and polarisation fields, alloy disorder also leads to valence band mixing effects, which impact the DOP and thus the LEE. The latter aspect is largely unexplored, as it requires 3D simulations in the framework of a multi-band electronic structure theory. Here, we study the DOP of (Al,Ga)N-based QW systems on the basis of an atomistic tight-binding model (TB). Special attention is paid to (i) the well width, (ii) Al content, and (iii) carrier density in the wells. Our calculations show that in terms of the DOP, in particular for high Al systems, wider wells can offer potential benefits to improve the LEE of such (Al,Ga)N light emitters.

II. Theoretical framework

To account for the impact of alloy disorder on the electronic and optical properties of (Al,Ga)N QWs, we employ the atomistic multi-band TB model introduced in Ref. [4]. The model is also coupled with a self-consistent Schrödinger-Poisson solver to account for carrier density dependent screening of internal polarisation fields. To cover TE and TM polarized light emitters, two QW systems have been targeted, namely $Al_{0.48}Ga_{0.52}N/Al_{0.63}Ga_{0.37}N$ for TE and $Al_{0.75}Ga_{0.25}N/Al_{0.9}Ga_{0.1}N$ wells for TM polarized light. The studies are carried out for different well widths and carrier densities. To gain insight into the impact of alloy disorder on the electronic structure, Urbach tail energies have been calculated [5], [6]. In terms of the DOP, we study the orbital character of the valence states [5].

III. Results

As the barrier has a higher AlN composition than the well, the emission characteristics of the QW will depend on how the hole states interact with the barrier material. As such, Fig. 1 shows the average probability of the hole charge density, $|\psi_h^{\text{AVG}}|^2$, confined inside the $Al_{0.75}Ga_{0.25}N$ QW as a function of energy and carrier density for a 1.3 nm wide well. The colour bar gives the orbital character of the different states. Here, blue indicate predominately p_z orbital character or TM polarization while yellow indicates predominately $p_x + p_y$ orbital character or TE polarization.

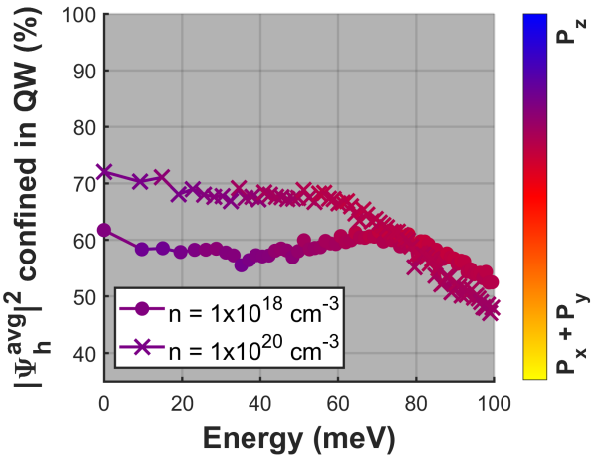

Fig. 1. Average probability of hole charge density, $|\Psi_h^{\text{avg}}|^2$, confined inside a 1.3 nm $Al_{0.75}Ga_{0.25}N$ quantum well as a function of energy. The data are averaged over 150 configurations. The average state energy is plotted with respect to the average ground state energy and for the carrier densities of $n = 1\times10^{18}$ cm^{-3} (circles) and $n = 1\times10^{20}$ cm^{-3} (crosses), respectively. The colour coding gives the averaged orbital contribution of each energy level (blue: p_z; yellow: $p_x + p_y$). Figure adapted from Ref. [5].

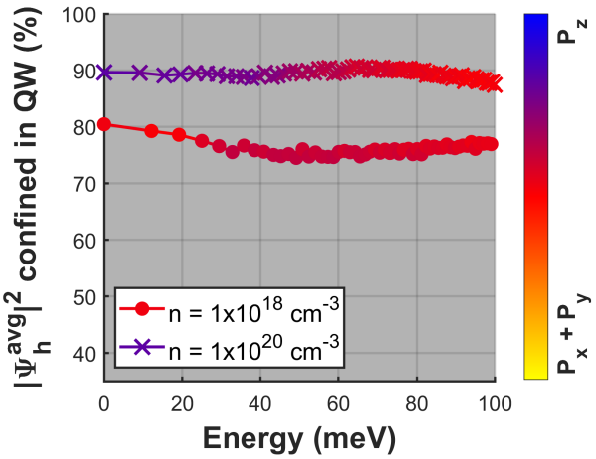

Fig. 2. Average probability of hole charge density, $|\Psi_h^{\text{avg}}|^2$, confined inside a 3.3 nm $Al_{0.75}Ga_{0.25}N$ quantum well as a function of energy. The data are averaged over 150 configurations. The average state energy is plotted with respect to the average ground state energy and for the carrier densities of $n = 1\times10^{18}$ cm^{-3} (circles) and $n = 1\times10^{20}$ cm^{-3} (crosses), respectively. The colour coding gives the averaged orbital contribution of each energy level (blue: p_z; yellow: $p_x + p_y$). Figure adapted from Ref. [5].

Figure 2 shows the data for a 3.3 nm wide well. These figures reveal that for the narrow well width of 1.3 nm, a width often used in deep UV (Al,Ga)N light emitters, the wave functions leak significantly into the barrier material. While this feature may be attractive for carrier transport between wells in multi QW systems, it may also lead to increased non-radiative recombination due to defects in the barrier material. With increasing carrier density, wave functions are more strongly bound in the QW. We attribute this effect to a screening of the built-in polarisation fields.

Increasing the well width has two benefits, it increases carrier confinement in the well and depending on the carrier density the orbital character tends towards p_x and p_y like states. However, with increasing carrier density more p_z like states become available. This observation also correlates with Urbach tail energies, which provide an indication for carrier localisation in the system. For the narrow QW, the Urbach tail energy affected very little by changes in the carrier density. In contrast, for wider wells the Urbach tail energy decreases with increasing carrier densities. This indicates that carrier localisation effects are strongly affected by the screening of the built-in field and as such so is the orbital character of the valence states. Thus, our calculations highlight an interplay of carrier density and well width on the electronic and ultimately optical properties of deep UV light emitters. Therefore, to improve TE polarised emissions and DOP in deep UV light emitters, wider QWs at lower carrier densities may be beneficial. The resulting increase in LEE would need to be balanced with other device characteristics such as radiative recombination rate which can decrease for wider wells.

IV. Conclusion

In this work, we investigated the electronic and optical properties of (Al,Ga)N-based QWs by means of an atomistic TB model. When coupled with self-consistent calculations, the impact of carrier density, well width and Al content on Urbach tail energies and the light polarisation characteristics of deep UV light emitters was studied. In terms of the degree of optical polarisation, our calculations indicate that wider wells at lower carrier densities can be beneficial for enhancing the light extraction efficiency of deep UV light emitters.

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