Atomistic analysis of transport properties of InGaN/GaN multi-quantum wells

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***Abstract*—We present an atomistic analysis of transport properties of an InGaN/GaN multi-quantum well system. Our study is carried out in the combined frame of tight-binding and Non-Equilibrium Green's Function theories. In our fully three-dimensional treatment, special attention is paid to the impact of random alloy fluctuations on the electron transmission probability. The calculations reveal that the alloy microstructure significantly impacts the transmission at least for the energetically lowest bound states in the quantum wells.**

***Index Terms*—InGaN, quantum wells, transport properties, atomistic description**

I. Introduction

III-Nitride materials, InN, GaN, AlN and their respective alloys, have attracted attention for producing high efficiency light emitting diodes (LEDs) covering, in principle, an emission wavelength range from ultraviolet to infrared [1]. Especially when targeting LED structures operating in the visible spectral range, InGaN-based quantum well (QW) structures are of central importance.

While InGaN-based emitters operating in the blue spectral range have found widespread applications, several fundamental phenomena which limit the device performance are not well understood. For instance, InGaN LEDs experience a so-called "efficiency droop" [2], which describes the effect that, as the current density in the device increases to operating densities, the external quantum efficiency decreases. This detrimental effect is more pronounced when pushing the emission to longer wavelengths, e.g. into the green spectral region [3]. Its fundamental origin is still under debate [2].

When addressing the transport properties of InGaN-based LEDs, idealized assumptions are widely made. For instance, these structures are often described in the framework of one-dimensional drift-diffusion equations [2]. In such models the InGaN alloy is treated as an effective medium that can be described by averaged material parameters, neglecting therefore the underlying alloy microstructure. However, several studies have shown that the alloy microstructure significantly affects electronic and optical properties on InGaN QWs [4], [5]. Only recently, three-dimensional (3-D) calculations including random alloy fluctuations in the framework of a modified drift-diffusion model have been reported, demonstrating the importance of an advanced theoretical treatment for an accurate description of transport properties of InGaN-based LEDs [6].

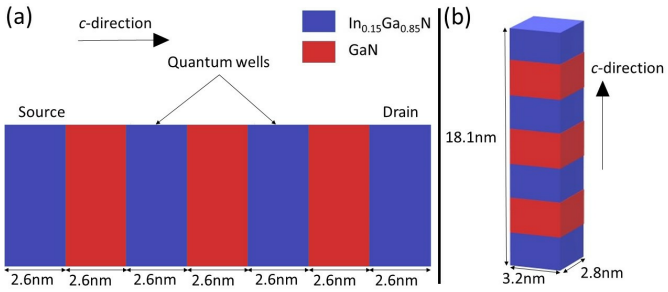

Fig. 1. (a) Side view of the model system. (b) Dimensions of the supercell used.

In this work we present a fully atomistic description of transport properties in InGaN/GaN multi-QW (MQW) structures. The electronic properties are treated by means of tight-binding (TB) theory and are described on an atomistic level. The TB model is then coupled to the Non-Equilibrium Green's Function (NEGF) solver OMEN [7] to investigate the impact of the alloy microstructure on the transmission/tunneling through a InGaN/GaN MQW system in a quantum mechanical picture. The results from a virtual crystal approximation (VCA) are compared with the outcome of calculations that account for random alloy fluctuations in the wells. Our results show that the transmission probability is significantly affected by random alloy fluctuations.

II. Theoretical Framework

Our electronic structure calculations are performed in the framework of a nearest-neighbour sp^3 TB model [5]. This allows us to capture the effects of varying atomic configurations within the different QWs constituting the MQW system, an information usually lost in "standard" 1-D models. As a test system we have chosen a MQW that consists of two 2.6 nm $In_{0.15}Ga_{0.85}N$ QWs separated by 2.6 nm wide GaN barriers. The in-plane dimension of the system is $\approx 3.2 \times 2.8$ nm^2 and the height of the supercell is ≈ 18.1 nm. To gain insight into the transmission properties of electrons, the system starts and ends with $In_{0.15}Ga_{0.85}N$, so that no dissipative process is required to populate the QWs with electrons. Overall, the

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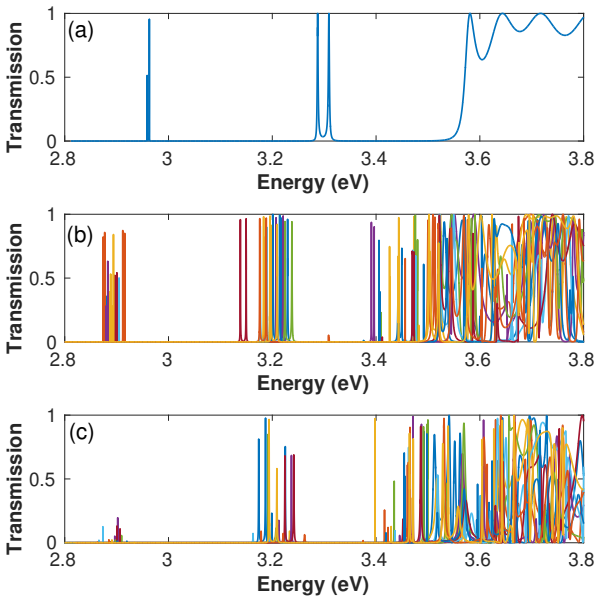

Fig. 2. Transmission through the InGaN/GaN MQW system shown in Fig. 1. (a) VCA. (b) System with the same random In configuration in each well. (c) System with different random In configurations in each well. For (b) and (c) results from 10 different microscopic configurations are displayed.

supercell contains $14,000$ atoms. A schematic illustration of the system is given in Fig. 1.

To determine the impact of (random) alloy fluctuations in the InGaN QWs on the transmission properties of the MQW structure, we have studied three different theoretical realizations of this system. First, a VCA is used for the $In_{0.15}Ga_{0.85}N$/GaN MQWs, thus neglecting the alloy microstructure in the calculations. Second, a random alloy treatment of the wells is applied, but the two QWs are generated to have the same atomic configuration. Finally the alloy microstructure is allowed to be different between the two wells. The In content is kept on average close to 15% as in the VCA. For the latter two microscopic descriptions, the calculations have been repeated 10 times to analyse the impact of the alloy microstructure on the results in more detail. To concentrate on the impact of random alloy fluctuations on the results only, built-in fields and (local) strain effects have been neglected initially.

III. Results

Figure 2 shows the transmission probability for electrons through the above discussed InGaN/GaN MQW systems. We start our analysis with Fig. 2 (a), which depicts the results of the VCA. We observe two doublets of sharp peaks below the GaN band gap ($E_g^{GaN} = 3.45$ eV). The double peak structure results from the fact that for the here considered barrier width an electronic coupling between the electron states in the two different QWs is found. The first doublet (≈ 2.97 eV) corresponds to the electron ground state while the second doublet (≈ 3.3 eV) stems from the first excited state in each well. Above 3.45 eV we observe the onset of the transmission through unbound/delocalized states.

Figure 2 (b) depicts the transmission through the two wells containing the same atomic configuration for 10 different microscopic configurations. This calculation clearly shows that random alloy fluctuations significantly affect the transmission properties of the system, given the wide spread in transmission peaks when compared to the four peaks in the VCA results below the GaN band gap (cf. Fig. 2 (a)). However, the overall trend of finding two large transmission probabilities (>0.4) in two distinct energy regions below the GaN band gap remains present in this atomistic description.

The situation changes significantly when the alloy microstructure in the two wells is different as Fig. 2 (c) demonstrates. Here, transmission stemming from the energetically lowest electron states in the QWs is strongly reduced. We relate this to the situation that electron ground states in two wells are now different and that the electronic coupling between these states is reduced due to carrier localization effects originating from the random alloy fluctuations in the wells. However, the transmission through the energetically higher lying states (around 3.2 eV) is similar to the results where the "randomness" in the two wells is the same. This indicates that the difference in the alloy microstructure between the two wells is of secondary importance in this energy range.

IV. Conclusion

We have presented an atomistic description of the transport properties in an $In_{0.15}Ga_{0.85}N$/GaN MQW system. Special attention was paid to the impact of random alloy effects on transmission probability, revealing that random alloy fluctuations can significantly affect this quantity. The here established framework presents a very good starting point for future investigations to gain detailed insight into the transport properties of InGaN/GaN LEDs on an atomistic level.

Acknowledgment

This work was supported by the Sustainable Energy Authority Ireland, Science Foundation Ireland (project no. 17/CDA/4789) and the European 7th Framework project DEEPEN (grant agreement no. 604416).

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