Effect of alloy fluctuations in InGaN/GaN quantum wells on optical emission strength

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***Abstract*—In this work we present the effect of compositional fluctuations in InGaN/GaN quantum wells (QWs) on their spontaneous emission properties. We show that random alloy fluctuations lead to fluctuations of both the optical matrix elements and the emission energy and that the two quantities are correlated. A qualitatively different behaviour between flat band QWs and QWs with strong quantum confined Stark effect is found and explained by the localization behaviour of electrons and holes.**

I. Introduction

Since the electrical energy consumption for lighting has been reaching a considerable amount and is now accounting for roughly 20% of total electric power consumption in Europe and USA, much effort has been dedicated to date to the development of efficient solid state lighting solutions based on LEDs. The currently most advanced material system for efficient LED lighting are the III-nitrides [1], [2]. One of the most interesting properties of InGaN in particular is that it covers the whole visible spectrum, allowing potentially all-nitride phosphor-free white LEDs [3], [4], [5]. The main advantage of such an RGB type approach consists in the elimination of the phosphor-based conversion, leading to potentially higher efficiency, increased lifetime and better color control.

The main limiting factor for reaching phosphor-free white LEDs based on RGB color mixing is the low efficiency of green and yellow/amber LEDs both in InGaN/GaN and AlInGaP technology, also known as the "green gap" [5]. InGaN/GaN based green and yellow LEDs require very high In fractions, leading to severe technological problems associated with high strain due to large lattice mismatch and to practical problems like strong quantum confined Stark effect (QCSE).

The origin of the strong decrease in efficiency when moving from blue to green with InGaN/GaN QW LEDs is still unresolved. In this work we study the spontaneous emission properties of InGaN/GaN QWs as one factor influencing LED efficiency. In particular we study the effect of alloy fluctuations on the optical transition matrix elements. It is known that random alloy fluctuations lead to fluctuations of the electronic band gap with FWHM of several tens of meV, increasing with In concentration [6]. Here we show that also the transition matrix elements statistically fluctuate. Moreover, we find that the amount of fluctuation and the statistical correlation with the band gap fluctuations strongly depend on the built-in electric field in the QW.

For our simulations we use an empirical tight-binding model (ETB) with $sp^3d^5s^*$ parametrization [7], implemented in the multiscale simulator tiberCAD [8]. To assess the influence of the statistical distribution of In atoms in the InGaN alloy, we drop the effective material approximation usually used in combination with the virtual crystal approximation (VCA). We assume that the random distribution of the In atoms is close to uniform [9]. For an adequate representation of the random alloys we use supercells in the QW plane of roughly 6×6 nm^2.

Since InGaN/GaN structures are highly lattice mismatched, strain has to be included in the tight-binding Hamiltonian, which is done by means of a Harrison scaling. Due to the random distribution of the In atoms and to correctly include internal strain, we use a modified Keating's valence force field (VFF) model to calculate elastic strain [10].

The simulated structures have been generated by randomly exchanging the Ga atoms in the QW volumes of a GaN crystal by In atoms. The total number of In atoms has been fixed so that the global mean In concentration is the same for every sample structure. The VFF and ETB calculations have then been performed for different nominal In concentrations on roughly hundred random samples per structure.

II. Simulation results

The model has been applied to 3 nm single QW LED structures including an AlGaN blocking layer. We first calculated the ground state transition energies and matrix elements for flat QWs with 15, 20 and 25% In. Flat band conditions have been achieved by excluding all polarization fields and dopings. Fig. 1a shows the scatter plot of the obtained optical matrix elements for roughly 20 random samples of each structure. It can be observed that the results considering a uniform random alloy lead to a fluctuation of both emission energy and transition matrix elements, with a clear correlation between the two quantities. The fluctuations of the matrix elements is in the order of 10 to 20%, and the mean values are 8–11% below the corresponding value obtained using virtual crystal approximation. Fig. 1b shows the corresponding results for the real QW, considering QCSE which leads to the well known spatial separation of electron and hole states along QW growth direction. In this case the fluctuation of the transition matrix elements is much stronger than in the flat band case,

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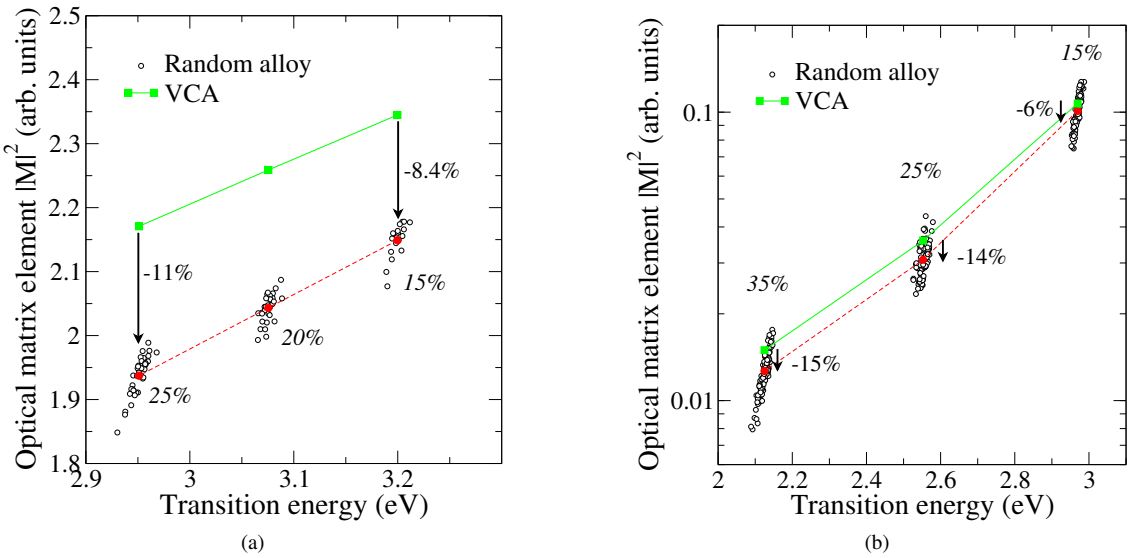

Fig. 1. Ground state optical transition matrix elements for 3 nm wide InGaN/GaN QWs, under flat band conditions for 15, 20 and 25% In (a), and considering QCSE for 15, 25 and 35% In (b). Square symbols show VCA based results, dashed lines with red filled symbols give the mean values of the random alloy data.

with roughly ±50%. This can be attributed to a fluctuation of the wave function overlap in the QW plane. In fact, due to the QCSE induced spatial separation of the carrier probability densities, electron and hole states are subject to compositional fluctuations in spatially different regions of the QW structure, leading to independent fluctuations of the probability densities in the QW plane for electrons and holes as shown in Fig. 2. Since this effect is not included in VCA based models, they overestimate the effective wavefunction overlap. As a result, a reduced spontaneous emission coefficient and thus a lower efficiency can be expected when compared to typical VCA based calculations, with a stronger discrepancy for higher In contents.

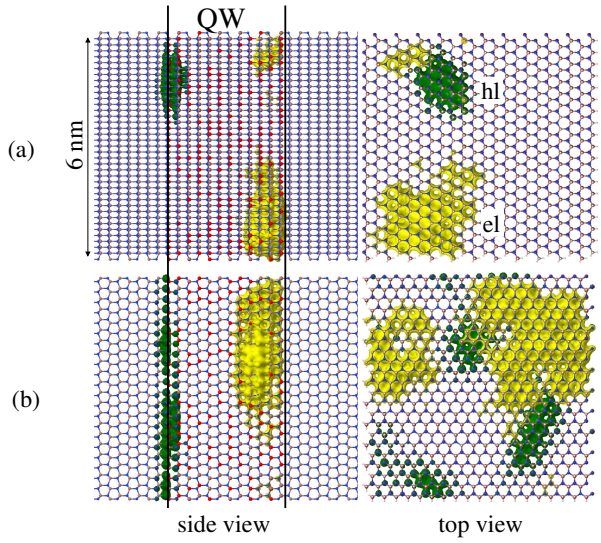

Fig. 2. Electron (yellow) and hole (green) probability density iso-surfaces for a 35% In QW with smallest (a) and biggest (b) optical matrix element. Both sideviews and top views are shown.

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