Simulation of Random Alloy Effects in InGaN/GaN LEDs

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***Abstract*—We present atomistic simulations of InGaN quantum disk and quantum well structures considering randomly distributed In atoms. It is shown that the random alloy fluctuations lead to an intrinsic broadening of the optical emission lines with an asymmetric tail towards long wavelengths. The amount of broadening is found to be dependent on In content.**

I. Introduction

Lighting accounts for roughly 20% of total electric power consumption in europe and USA. Therefore, in the last decades considerable effort has ben put into the development of highly efficient white light sources such as LEDs. One of the most promising material systems for solid state lighting is InGaN/GaN [1], [2]. InGaN potentially covers the whole visible spectrum and would thus theoretically allow for all-nitride phosphor-free white LEDs [3], [4], [5]. However, several issues in the growth of InGaN/GaN systems have prevented so far from reaching both maximum efficiency and good color rendering index (CRI). In particular, the handling of high elastic strain due to large lattice mismatch, strain relaxation effects in 3D structures like nanorods, high internal electric polarization fields and Indium concentration fluctuations are challenges that have to be addressed in order to further increase LED efficiency.

In this work, we study the influence of random alloy fluctions on the fundamental transition in InGaN/GaN quantum dots (QD) and wells (QW). We assume that the random distribution of the In atoms is close to uniform [6], [7]. For the simulations we use an empirical tight-binding model (ETB) with $sp^3d^5s^*$ parametrization [8], implemented in the multiscale simulator tiberCAD [9]. Usually, calculations of optoelectronic properties of alloys are based on the virtual crystal approximation (VCA), which defines an effective material by linear or quadratic mixing of the constituents' parameters. To assess the influence of a random disposition of In atoms in the InGaN alloy, we drop the effective material approach and use for each pair of atoms the parameters of the corresponding bulk material, InN or GaN.

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

The simulated structures have been generated by randomly exchanging the Ga atoms in the QD or 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 was the same for every sample structure. The VFF and ETB calculations have then been performed for different nominal In concentrations on several hundred random samples, and the resulting statistical dataset for the ground state transition energies has been analyzed.

II. Simulation results

The VFF/ETB approach used for the simulations has first been validated for random alloy bulk InGaN. The results are in good agreement with Density Functional Tight Binding (DFTB) calculations and with the experimental bowing of the band gap (see Fig. 1).

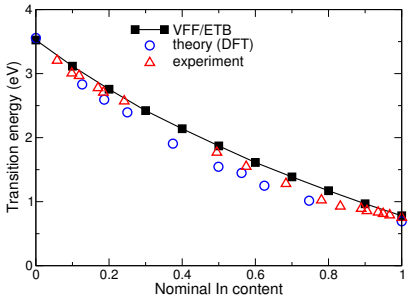

Fig. 1. Energy gap versus In concentration for bulk InGaN. Red triangles are experimental results.

The model has then been applied to a 2 nm thick QD in a hexagonal GaN nanocolumn of 13 nm diameter. Fig. 2 shows the ground state transition energy both using VCA and random alloy models. It can be seen that VCA with linear interpolation considerably overestimates the transition energy. The statistical broadening of the peak emission energy, represented by the error bars, increases with increasing In concentration. The mean value of the emission energy shows approximately the same bowing as the bulk band gap.

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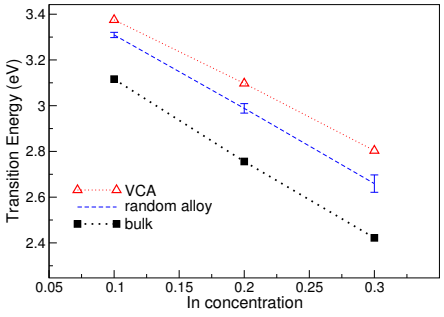

Fig. 2. Ground state transition energy resulting from VCA and random alloy based calculations. The bulk band gap is given for comparison.

Fig. 3 shows the spectra for the statistical ensemble (the sum of all single sample spectra) compared to a single sample emission for 10% and 30% In. The single sample spectra are taken as Lorentzians with 7 meV broadening centered at the sample's fundamental transition energy. We can deduce a random alloy induced broadening of 11 meV and 19 meV for 10% and 30% In, respectively. These values compare well with experimental results at low temperature [11]. Interestingly, increasing In content leads to increasing asymmetry of the spectrum, due to an asymmetry of the transition energy distribution.

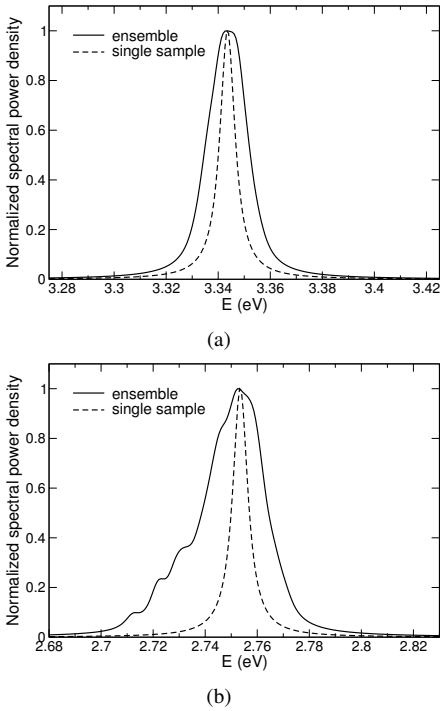

Fig. 3. Ensemble and single sample spectra for (a) 10% and (b) 30% In. The single sample spectrum is a Lorentzian at the mean emission energy.

We calculated the correlation between the transition energy and an effective In concentration. The latter has been calculated as weighted mean value of the local In concentration, using as weight the electron ground state spatial probability density: $x_{\mathrm{eff}} = \int c(r)|\psi(r)|^2 \, \mathrm{d}r^3$. The local In concentration $c(r)$ has been approximated as the mean concentration inside spheres of 5 Å radius. x_{eff} can be interpreted as the local effective In concentration seen by the electrons in the ground state. This value is indeed found to be correlated with the ground state energy, as can be seen in Fig. 4.

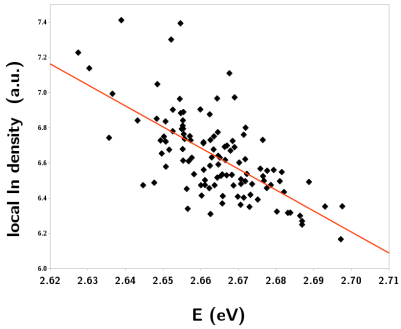

Fig. 4. Correlation between effective local In concentration and transition energy.

ACKNOWLEDGMENT

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