Designing microstructures for bandgap manipulation of InGaN Quantum Wells by **k.p** simulation coupled with molecular dynamics

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***Abstract*—In this work, we present the design of InGaN microstructures by manipulation of quantum well bandgap via strain engineering. By coupling strain field extracted from molecular dynamics simulation to k.p simulation, we are able to associate the effect of geometry and strain of a structure to its light emission.**

Keywords—III-Nitride, Quantum wells, Molecular Dynamics

I. Introduction

Coming to the age of nanotechnology, there is a trend of miniaturization to micrometer and nanometer size for optoelectronic and photonic devices. Miniaturization naturally increases light extraction efficiency [1], but more importantly, photonic devices exhibit unique physical properties within this mesoscopic regime that enables technologies such as photonic crystal [2], plasmonic nanostructures [3] and semiconductor nanowires [4] for integrated photonic circuits, bio-sensing and photovoltaics. In context of optoelectronics, miniaturization not only increases quantum efficiency [5, 6], but also inspires various novel applications, including tuning of emission color [6, 7] and custom design of band profiles [8]. Despite achieving different goals, these mesoscopic optoelectronic devices are all based on the same principle – tuning of the bandgap or band profiles via manipulation of quantum-confined Stark effect (QCSE) by strain engineering.

The most fundamental manifest of strain-induced spectral shift phenomenon for III-Nitride based devices is a spectral shift of photoluminescence (PL) after a reduction in dimension [5, 9], which is usually attributed to the strain relaxation of the multiple quantum wells (MQWs) due to sizing [5, 9-11]. There is general consensus that the MQWs would be able to relax the strain induced by lattice mismatch towards the sidewalls after sizing, resulting in a decrease in the piezoelectric polarization field inherent in *c*-plane wurtzite nitride devices and thus a reduction in the QCSE [11], leading to a blue-shift in the PL spectrum originating from the edge of the device.

However, there has been little investigation and explanation in the spatial distribution of the emission wavelength in relation to the strain field of a micro-/nano-structure. An earlier study [10] explained qualitatively that the emission wavelength can be affected by strain due to an interplay between QCSE and deformation potential. This seems to suggest that there are multiple factors affecting the mechanism of strain-induced spectral shifts.

Therefore, here in this work, we present on a computational approach to investigate the effect of strain field on bandgap on quantum wells in micro-/nano-structures. Molecular dynamics are employed to simulate the strain profiles of micropillars. The approach can more accurately model the lattice-mismatched coherent interface and strain-relaxed surfaces than conventional finite element method (FEM) as used in previous studies [12]. The underlying mechanisms of the dimensional-dependent spectral shifts can be better understood, which are crucial for the development of novel strain-engineered devices of micro-/nano- scale.

II. Simulations

2D molecular dynamics simulations are performed using *LAMMPS* [13] with a Stillinger-Weber potential for InGaN [14, 15]. The GaN block is fixed at the bottom ($y = 0$) with a compressive strain of 0.023% to emulate a boundary that is lattice-matched to a partially relaxed GaN buffer with a biaxial stress of 1 GPa. The computational domain is reduced to half a 2 μm-diameter micropillar, i.e., a dimension of 1 μm × 1 μm, by using a symmetric boundary, which restricts the lateral movement of the atoms, is imposed on one side of the block. 15 pairs of QWs are implemented such that the

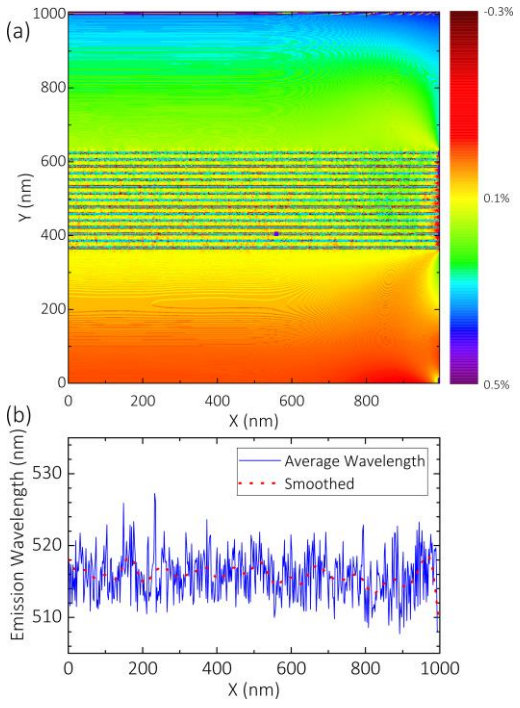

Fig. 1. (a) Out-of-plane strain field of a micropillar extracted from molecular dynamics simulations, and (b) the corresponding calculated emission wavelength

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InGaN wells have 18% Indium content and ~4.7 nm (9 atomic layers) of thickness, while the GaN barriers have a thickness of ~13.5 nm (26 atomic layers). The InGaN layers are initialized to be lattice-matched to the GaN layers, and are implemented as a random alloy, i.e., the Ga atoms in the wurtzite structure is randomly replaced with Indium atoms within the supposed InGaN quantum well regions, with the proportion of In atoms satisfying the estimated Indium content for the quantum wells. The structure is then subjected to an energy minimization to relax the atomic positions

Subsequently, the strain field extracted from the molecular dynamics simulation is included in the **k·p** perturbation theory to solve the Schrödinger equation, according to the steps described in [16-18]. For each point of calculation, a locally averaged Indium composition is also used instead of using a single value of Indium composition for all positions in all QWs.

III. Results and Disucssions

Fig. 1(a) shows the out-of-plane strain field as extracted from molecular dynamics simulations. The micropillar exhibit a relaxation of the MQWs at the edge (X = 1000 nm) as expected. When the micropillar relaxes as a whole, the lattice-matching interface will then try to maintain the lattice arrangement, thus increasing the out-of-plane tensile strain at the edge as shown in Fig. 1(a). The composition fluctuation of the InGaN well layers due to the nature of random alloy also results in fluctuation of the strain field.

Fig. 1(b) shows the calculated emission wavelength, using the strain field from molecular dynamics in the **k.p** calculations. As can be seen, the fluctuation in InGaN well strain as a result of the Indium composition fluctuation causes a fluctuation of the emission wavelength. We can also observe that there is a significant blue-shift at the edge of the micropillar at the edge due to strain relaxation.

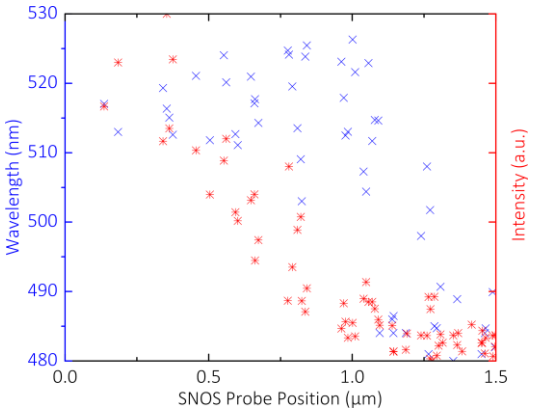

Fig. 2. Near-field PL line profile of a 2 μm-diameter micropillar measured by SNOS

Fig. 2 shows near-field photoluminescence (PL) measurement by Scanning Near-field Optical Spectroscopy (SNOS). The experimental measurement demonstrates similar fluctuation in emission wavelength and sharp blue-shift near the edge of the micropillar.

Detailed results and comparison of micropillars with different Indium composition are published in [19].

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