Random alloy fluctuations effects on the spontaneous emission properties of a InGaN/GaN LED

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Abstract—A theoretical study based on an empirical tight-binding model is presented regarding the effect of random alloy fluctuations on the spontaneous emission properties in the quantum well of an InGaN/GaN LED.

Keywords— LED, InGaN/GaN, Tight-binding;

I. INTRODUCTION

A notable effort in order to produce efficient and less consuming light sources has been pursued in recent years since lighting has become one of the major causes of global energy consumption, an effort that has been heavily focused in the development of sources based on inorganic light light-emitting diodes (LEDs) [1].

In the last two decades a relevant role in the fabrication of LEDs has been played by alloys containing Indium Gallium Nitride (InGaN) [2–4], since by In content engineering in the active region it is theoretically possible to cover the whole visible spectrum range [5-6].

By using atomistic approaches it is possible to model in detail realistic indium distributions including local strain fields in order to obtain more accurate electronic calculations as well. In this work we present a theoretical study of the effect of random alloy fluctuations on the spontaneous emission properties in the quantum well (QW) of an InGaN/GaN LED.

II. METHODOLOGY AND RESULTS

Our calculations are based on an empirical tight-binding (ETB) model, using an sp3d5s* parametrization [7-8]. Strain is calculated with a valence force field (VFF), preconditioned with a continuous linear elasticity model [9]. The devices consists of a single 3 nm QW with varying In content, undoped GaN barriers and AlGaN EBL. As a first step a selfconsistent solution of the Schroedinger drift-diffusion model at a realistic operating current is determined using a k*p model [10]. Then we calculate the first few electron and hole states using ETB, and from these states the correspondent optical matrix elements. These calculations are repeated for a statistical ensemble of structures with uniform random In distributions in the QW for each mean In concentration. A periodic supercell in the plane of the QW of 6x6 nm² has been implemented in order to have a reasonable representation of the random alloy and of the induced fluctuations of the particles orbitals. This results in a statistical distributions of the transition energies and oscillator strengths for different In concentrations. Our results show that the oscillator strengths are correlated with the transition energy, and that the mean oscillator strength of the random alloy calculations presents a stronger decrease with In concentration than the one usually obtained using virtual crystal approximation.

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REFERENCES