Coupling Drift-Diffusion/NEGF for the Simulation of InGaN/GaN LEDs

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INTRODUCTION

The InGaN/GaN is currently one of the most promising material systems for the development of high efficiency white light sources and has therefore attracted much attention in the last years [1]. Since InGaN potentially can cover the whole visible spectrum, a phosphor-free all-nitride white light source is theoretically possible [2,3]. Still, there are two main challenges faced by the development of high power white InGaN/GaN multi quantum well (MQW) LEDs. The first one is a severe efficiency droop with increasing operation current [4], and the second is a systematic drop of the peak external quantum efficiency (EQE) with increasing In content, i.e. increasing emission wavelength [2]. The origin for both effects is currently not completely understood. Besides nonradiative recombinations, carrier leakage and poor carrier injection into the active layer may play a role. Due to the spontaneous and piezoelectric polarization fields, InGaN/GaN MQW structures show strong built-in electric fields and significant injection barriers. In this work, we study the carrier transport through injection and inter-well barriers, and tunneling across electron blocking layers by means of non-equilibrium Green’s functions (NEGF) [5], based both on continuous kp and atomistic empirical tight binding (ETB) parametrizations and coupled in a multiscale/multiphysics fashion to a semi-classical drift-diffusion transport calculation [6].

DISCUSSION

For the calculations we consider a typical InGaN/GaN MQW structure with 5 QWs and an AlGaN/GaN blocking layer after the active layers. Since we are mostly interested in green LEDs, we assume an In content of 25%. Fig. 1 shows the band structure resulting from a semi-classical drift-diffusion calculation for an applied bias of 2.6 V, corresponding to roughly 10 mA/cm^2. Usually, drift-diffusion based calculations overestimate the knee voltage of nitride LEDs due to the internal voltage drop at the injection and inter-well barriers, as can be seen in the figure. To have a more accurate description of transport across the barriers, we calculate the ballistic current using NEGF. Here we assume a barrier with 5% In content. For comparison, we calculate the current both for a kp and a full-band ETB parametrization. The latter moreover allows to assess the effect of the randomly distributed In atoms in the barrier. In Fig. 2 we show a close-up of the conduction band profile of the relevant device part and the transmission using kp single band, kp 8x8, ETB with virtual crystal approximation (VCA) and several ETB results with uniform random alloy distributions (RND). These lead to considerable fluctuations in the transmission function, giving a distribution in the effective barrier resistivity in the range of 0.28 – 1.26 Ωcm^2, compared with 0.47 Ωcm^2 of VCA and 1.33 of EFA 8x8. These values are considerably lower than the resistivity of 6.9 Ωcm^2 extracted from the drift-diffusion result, and are in the range of values needed to fit experimental IV curves.

In Fig. 3 we show the transmission across the $Al_{0.15}GaN$ EBL, calculated based on ETB using VCA (triangles) and random alloy (red lines). Also in this case the randomly distributed atoms lead to an increase in the ballistic transmission because of mechanisms that closely resemble defect-assisted tunneling.

ACKNOWLEDGEMENT

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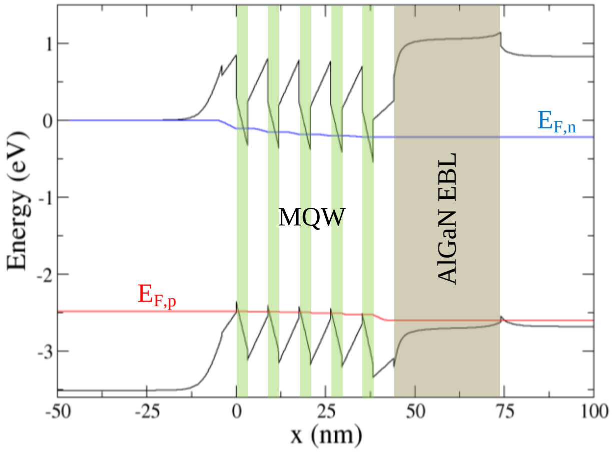

Fig. 1 Band diagram of the simulated InGaN/GaN LED.

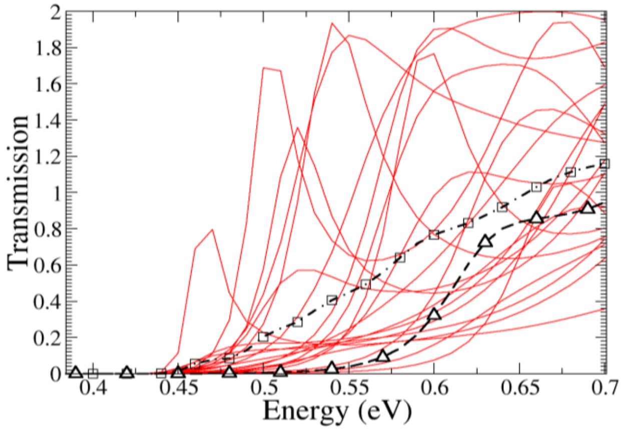

Fig. 3 Transmission across AlGaN EBL. Triangles: VCA, red lines: random alloy, square: mean of random alloy results.

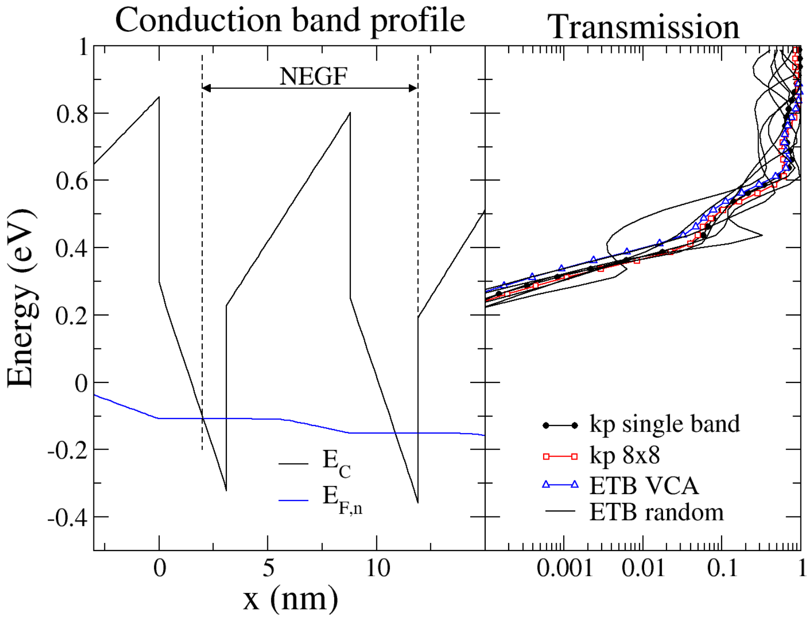

Fig. 2 Close up of the quantum mechanically treated part and transmission for the different models.