Numerical modelling of non-planar GaN LED with CNT top contact

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Abstract. In this paper, the theoretical study of LED based on GaN NWs with carbon nanotubes (CNT) top contact has been presented. The main electrical and optical characteristics of LED have been numerically calculated. In a 0.5 x 0.5 mm NWs array, the Ohmic losses in CNTs were 2.7% with an operating current density of 50 A/cm². It proves the possibility of using CNTs as transparent contact.

1. Introduction
In the last decades, III-Nitrides attract attention as materials for optoelectronic devices due to their outstanding properties. AlN, GaN, and InN and their alloys have a direct bandgap varied from 0.7 eV to 6.2 eV [1]. It allows producing light emission diodes (LEDs) with a broad range of emitted wavelengths.

Recent progress in the development of wearable and bio-compatible devices faced a challenge to get stretchability and flexibility of electronics and, in particular, LEDs. These properties can be achieved with III-Nitrides by a transition from conventional planar geometry to 1D structures such as nanorods or nanowires (NWs) [2].

Using NWs solves many inherent problems of thin-film LEDs. Firstly, dislocation density declines in GaN nanowires with a high surface-to-volume ratio. Also, the more intensive strain relaxation was observed in comparison with planar GaN, which led to decreasing internal electrical fields induced by lattice mismatch with traditional substrates such as sapphire and Si [3]. Secondly, such structure changes suppress the waveguide effect on interfaces GaN/air (n=2.4) and promote light extraction [4]. Moreover, such geometry gives additional advantages, the main of which is the ability to control a radiation pattern [5] and wavelength of emitted light [6] by changing the structure sizes and shape.

To take all advantages mentioned before, the contacts to a LED should be transparent and retain their properties upon deformation. The literature reports on the use of conductive composites (silver nanowires/nanoparticles [7] or reduced graphene oxide penetrating into an elastic polymer [8]), woven conductive fibers/filaments [9], ionic hydrogels [10] and liquid metal as stretchable electrodes [11]. However, all of these solutions have their drawbacks. The resistance of silver nanowires increases dramatically when stretched due to the high Young’s modulus. Reduced graphene oxide also loses its...
conductivity as it stretches. Some ionic hydrogels have good stretchability, but insufficient electrical conductivity can result in poor device performance. The gallium-based liquid metal exhibits excellent tensile and recyclability, however, it is extremely susceptible to oxidation and has a high surface tension, which affects its fluidity and makes it difficult to use in nanoscale systems.

Carbon nanotubes (CNTs) can be considered as rolled nanowire graphene sheets, combining the advantages of graphene and silver nanowires, providing low cost, production scalability, ease of use, and improved current collection [11]. The latter properties, together with antireflection characteristics and high stability, make CNTs one of the most promising transparent flexible and extensible contact materials. Despite the fact that the literature contains data on preliminary studies of CNT layers in optoelectronics, their potential has not yet been fully disclosed. This last statement is especially true for high performance stretchable LEDs based on GaN NWs. Therefore, this work is devoted to the numerical modeling of GaN NWs-based LED with CNT top contact to determine its optoelectronic characteristics.

2. Modeling
The considered LED is an array of axial heterojunction GaN NWs with inserted InGaN quantum well. In this system, the current flows mostly vertically due to the geometrical restriction. Thus, each NW separately could be modeled as a 1D structure instead of 3D or 2D with axial symmetry. The modeled NWs contain the n-doped GaN bottom barrier, InGaN quantum well, undoped GaN top barrier, p-doped AlGaN layer, and p-doped GaN.

In the area of InGaN quantum well, the Schroedinger-Poisson equation has been solved to determine the density of states in the quantum well and calculate charge tunneling through it. The modeled energy diagram is presented in Figure 1.

![Figure 1. Band diagram of the NWs active area.](image)

Also the current-voltage characteristic and emission spectra of a single NW have been obtained in the calculation process. The calculated at different voltages light emission spectra are presented in Figure 2. It have a maximum power density at the wavelength of 459-460 nm, which matches with experimental data [12].

In the next step, an array of NWs has been modeled by integrating currents over the surface, taking into account the optical losses in the CNT layer. The voltage drop in the CNT was taken into consideration to calculate the dependency of current flows through the NWs on coordinate. The resulting currents spreading in CNT are presented in Figure 3. The Joule heat was calculated by the
Ohm laws using the obtained current distribution. The 0.5×0.5mm CNT layer generates heat of 15.4 mW. The input power was calculated from applied voltage and integrated current. Based on the previous data, we calculated relative Ohmic losses in the CNT layer, which were 2.7% at the current density of 50 A/cm².

Figure 2. Photoluminescence spectra for the different applied voltages.

Figure 3. Distribution of currents in the CNT layer.

3. Conclusions
The numerical model of GaN NWs-based LED with CNT contact has been implemented. The main characteristics of LEDs have been obtained. The calculated at different voltages emission spectra show a maximum power density at the wavelength of 459-460 nm. In a 0.5×0.5 mm NWs array, the Ohmic losses in CNTs were 2.7% with an operating current density of 50 A/cm². The obtained results demonstrate the possibility of using CNTs as a material for contacts to NWs LEDs.
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