Characterization of GaN-based quantum nanowire and resonant tunneling diode by simulations

Mohammed Nadir
Tampere University
Faculty of Engineering and Natural Sciences
Korkeakoulunkatu 6, FIN-33720 Tampere, Finland
email: mohammed.nadir.fi@ieee.org

Simulations are performed for wurtzite GaN nanowire in order to investigate electronic properties which influence the optical properties. The confinement potential and energies are achieved. The 6/8-band **k·p** method is used for electronic structures. Quantum wire could also manifest dark exciton. Simulations make use of dispersion relations. The resonant tunneling diode has also been calculated using multi-scattering Büttiker(MSB) probe for GaN/AIN structure wherein scattering mechanism has also been incorporated. The remaining parameters are varied in order to obtain the right structure and the plane of growth in GaN crystal.

Keywords: Quantum nanowire, resonant tunneling diodes, quantum transport, GaN wurtzite crystal, **k·p** method, qubit.

Enormous progress has been made in the development of GaN-based semiconductor concerning quantum wire (QW) and resonant tunneling devices (RTD) during the last decade. It has become very important structure in the field of low-dimensional physics and chemistry. Semiconductor quantum wires exhibit novel electric and optical properties owing to their one- dimensional structure and possible quantum confinement effects in two dimensions. GaN-based (wide-bandgap) quantum wire have a surpassing properties as compared to quantum well structures [6] and has earned a special place in optoelectronic devices. However, its wurtzite (hexagonal) structure, which leads to strong piezoelectric and pyroelectric field in polar heterostructures, see Fig. 1, e.g., $20\bar{2}1$ plane is suitable for yellow-green wavelength for the emission in semiconductor laser devices [1]. Different planes of heterojunction give creative way of studying internal polarization fields [2]. Therefore, GaN-AlN based resonant tunneling diode has been calculated by using a new method known as multi-scattering Büttiker (MSB) probe model, initiated in [10]. A double barrier resonant tunneling diode revived for studying internal spontaneous and piezoelectric polarization fields in polar heterojuntions, *i.e.*, tunneling transport within GaN-AlN heterostructure is influenced by spontaneous, piezoelectric and pyroelectric polarization. RTD is also good candidate for negative differential conductance [2].

A GaN (wurtzite structure, Fig. 1) nanowire is of cylindrical shape of radius 2 nm is simulated with infinite barrier so that wave function can be assumed to be zero at the boundary. In the nanowire with radius 2 nm, the electron-hole transitions (e1-h1) are not very probable because wavefunctions do not overlap much [4], *i.e.*, ground state of electrons $L = 0$ to ground state of holes

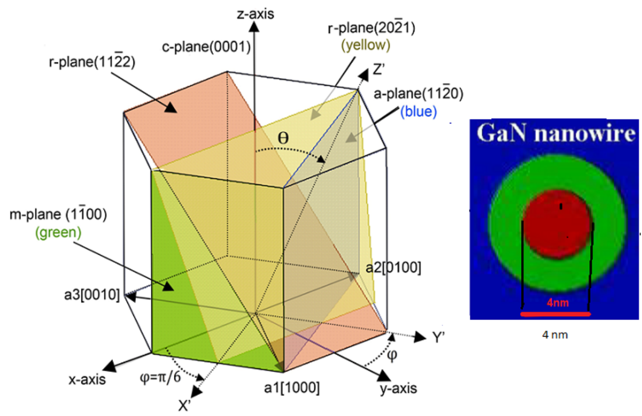

FIG. 1: Different planes are shown within GaN wurtzite crystal and depicting the nanowire of 4 nm diameter.

$L = +/-1$ (dark exciton effect [5]). Due to symmetry, some of the hole state are degenerate, however, three hole states are shown as probability density distribution, $|\psi(r)|^2$ in Fig. 3 while Fig. 2 is showing hole states as valence bands.

The resonant tunneling diode with two barriers of AlN consists of the following layers: GaN (5 nm thick, $7 * 10^{18}$ per cm^3 doping), GaN (2 nm thick, no doping), AlN (0.5 nm, no doping), GaN (4 nm thick), AlN (0.5 nm, no doping), GaN (2 nm thick, no doping), GaN(5 nm thick, $7 * 10^{18}$ per cm^3 doping) consecutively. Its density of states at the source and drain are shown in Fig. 4 and Fig. 5 respectively. This work is based on using the Nextnano software [3] and the publications as cited below [4, 6, 8, 9]. The results calculated by Nextnano match well with other groups [4]. The software has a vast variety of 'input files' (commands) which could be

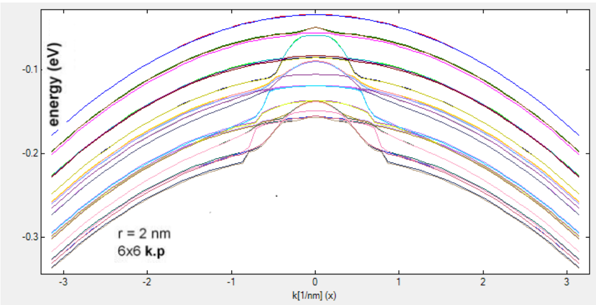

FIG. 2: Hole states of the cylindrical GaN nanowire and showing the dispersion near $k = 0$, which is possible reason for dark excitons.

adjusted in order to predict more realistic results.

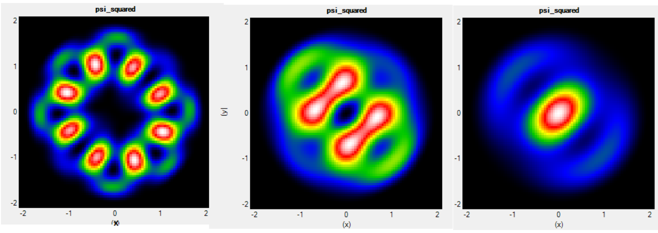

FIG. 3: Probability density distribution, $|\psi(r)|^2$, x & y in *nm*,, for the three hole states, namely 34th, 11th and 5th in the GaN nanowire.

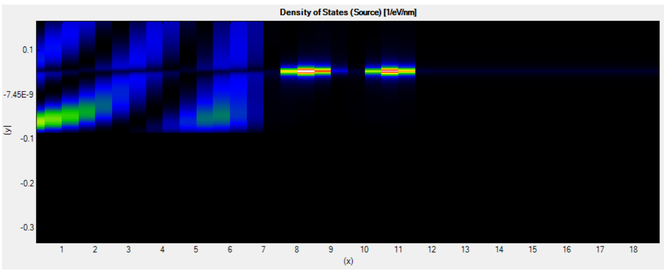

FIG. 4: Position resolved density of states at the source of RTD.

GaN-based nanowire with 4 *nm* diameter with infinite length has been investigated and an attempt is projected to realize dark-exciton which could act as a qubit. Making use of dark-exciton as qubit needs further innovations in order to predict theoretically and be compatible with experiments. During the last three years GaN-based RTD has made new advances [2] within the GaN-based family of semiconductors following its recognition in blue emission. Simple double-barrier III-nitride RTD shows how internal polarization fields can be studied. Herein the tunneling transport is strongly influenced by the internal spontaneous, piezoelectric and pyroelectric polarization fields which are inherent to the non-centrosymmetric

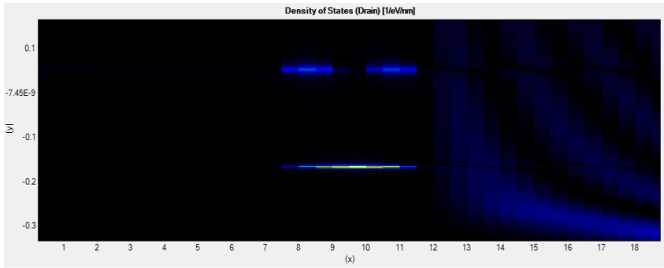

FIG. 5: Position resolved density of states at the drain of RTD.

crystal structure of III-nitride semiconductors. Its new application to build reproducible quantum cascade radiation has been observed at higher temperature, i.e., a new field of research [2, 8]. Multi-scattering Büttiker (MSB) probe method for quantum transport is also more computationally efficient as compare to nonequilibrium Green function method [9].

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[1] Nadir M, 'Selecting the right growth-plane within GaN Crystal for InGaN based Yellow Green or Yellow Lasers by Siinulations'.*Postdeadline poster MPD4342 at NUSOD 2014*, see http://www.nusod.org/2014.

[2] Xing H G, *et al.*, New physics in GaN reonant tunneling diodes. *Proceedings Volume 10918, Gallium Nitride Materials and Devices XIV; 109180Z (2019) https://doi.org/10.1117/12.2512638,* Event: SPIE OPTO, 2019, San Francisco, California, United States.

[3] http://www.nextnano.com.

[4] Zhang X W, Xia J B, 'Optical properties of GaN wutrzite quantum wires', *Journal of Physics: Condenced Matter* , 18 (2006), 3107-3115..

[5] Poem E *et al.*, 'Accessing the dark exciton with light' *Nature Physics online published:* 7 November 2010.

[6] Harrison P, Valavanis A, 'Quantum Wells, Wires and Dots', *Wiley*, fourth edition 2016.

[7] Greck P. 'Efficient calculation of dissipative quantum transport properties in semiconductor nanostructures', PhD thesis, Technische Universitat München, 2012.

[8] Greck P. *et al.*, Optics Express, Vol.23, No. 5(2015).

[9] Greck P. *et al.*,'The nonequilibrium Greens functions method and descendants: Ways to avoid and to go'.*' 2010 14th International Workshop on Computational Electronics. doi:10.1109/iwce.2010.5677996'.*

[10] Büttiker M. Phys. Rev. Lett. 57, 1761-1764 (1986).