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Atomistic Modeling of GaN Based Nanowires

L. Prokopova, M. Persson, M Povolotskyi, M. Auf Der Maur and A. Di Carlo*
Dept. Electronic Eng. University of Rome "Tor Vergata", via del Politecnico 1, 00133 Roma (Italy)
*e-mail: aldo.dicarlo@uniroma2.it

Recent progress in growth technology gives a possibility to produce high quality nitride nanostructures such as free-standing nanowires, quantum discs and quantum dots [1]. The growth of GaN nanotubes is of particular interest due to the large band gap of GaN. Potential applications of the structures are possible candidates for LEDs, Bragg reflectors, laser and photonic crystals, biochemical-sensing. The use of nanowires and possibly nanotubes as active components promise to enhance the performance of such devices due to increased charge localization and reduced defect density. We report a theoretical study of the electronic and optical properties of GaN wires and GaN/AlGaN heterostructures and of single crystalline semiconducting GaN nanotubes using an atomistic tight binding approach.

MODEL AND RESULTS

We consider two different kinds of objects: strain-free homogeneous GaN nanowires and pseudomorphically grown GaN discs embedded into a AlGaN column.

The GaN nanowire is modeled as an infinitely long oriented along the [0001] direction, with a hexagonal cross-section and wurtzite crystal structure. Both solid nanowire and hollow nanowire (nanotube) are considered. The calculations are based on an sp3d5s* nearest neighbor tight binding basis. The effect of introducing a hole in an nanowire is studied and we find that the charge in energy for the original nanowire states depends strongly on the state of the wave function. The first conduction band state increase in energy as the outer size of the nanotube is increased while keeping the tube wall constant. The order of the first two valence bands are reversed compared to the solid nanowire (Fig.1-2). For the optical properties we find that the transition between the first conduction band and first valence band is weak and that the first strong transition is associated with the second or third valence band. The lowest conduction band state is found to increase in energy as the radius of nanotube is increased. The first strong transition has a strong polarization anisotropy with the dominating component along the nanotube axis. A typical band structure for a solid GaN wire is shown in figure 3

Tight-binding calculations are also extended to AlGaN/GaN nanowires (see Fig 4) forming confining quantum disc. These structures are similar to those analyzed in Ref. [1]. Here piezoelectric as well as pyroelectric polarization have been accounted for by using a continuum model solved via the finite element method. The atomic position are relaxed by minimizing the elastic energy and the strain of the structure is calculated (Fig 5). From the strain map, the polarization vector is extracted and the potential profile is then obtained by solving the Poisson equation. The potential profile is shown in Fig. 6. Relaxed atomic position and potential profile are then feed back in the tight-binding solver and both electronic and optical properties of the AlGaN/nanowire are calculated. A detailed comparison between theory and experiment will be shown

ACKNOWLEDGEMENT

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REFERENCES

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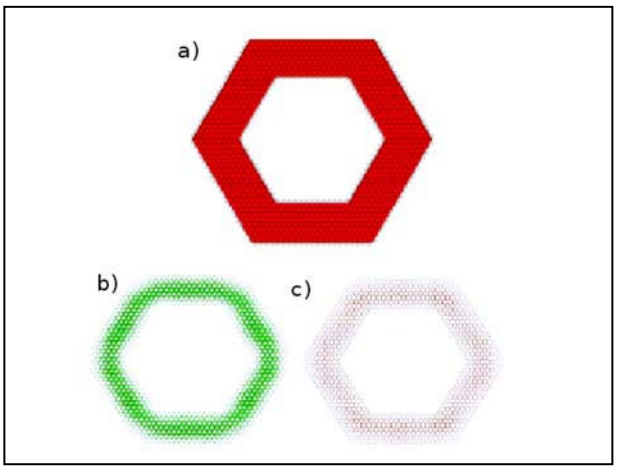

Fig. 1. (a)GaN nanotube (b) Second valence band state (c) First conduction band state

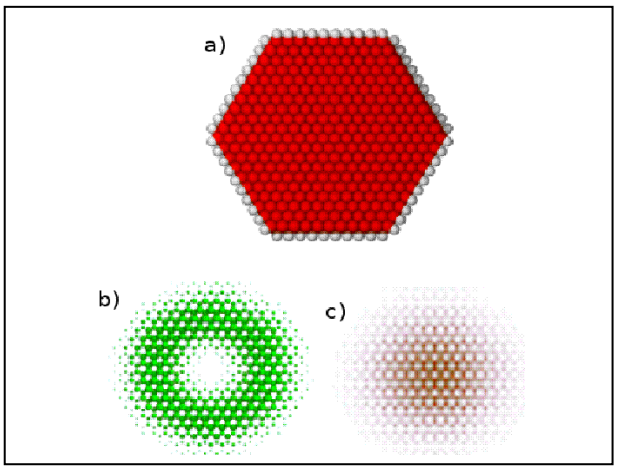

Fig. 2. (a)GaN nanowire (b) Second valence band state (c) First conduction band state

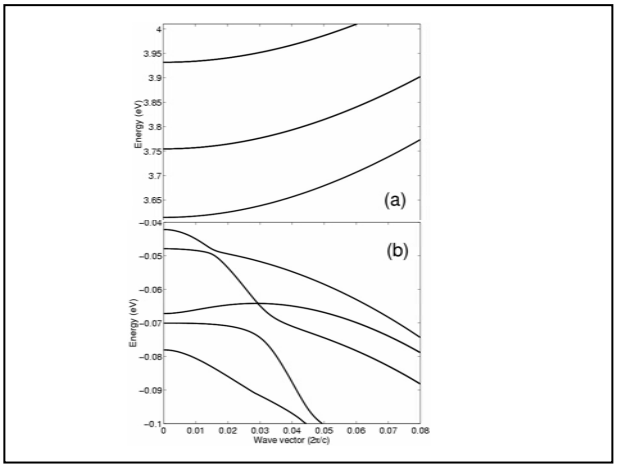

Fig. 3. Band structure of a solid GaN nanowire with 4.8 nm diameter. (a) conduction band (b) valence band

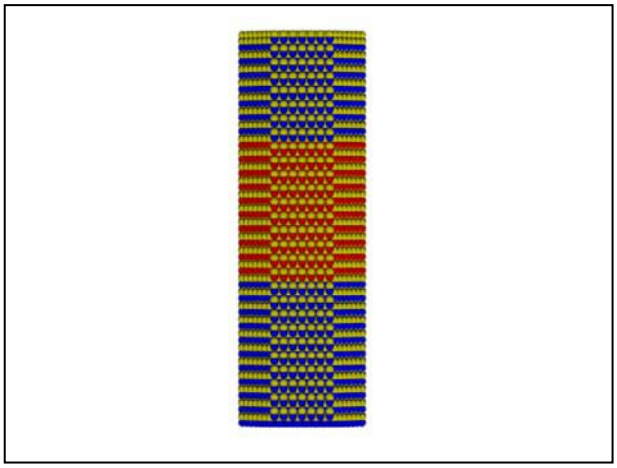

Fig. 4. Typical AlGaN/GaN nanowire used in the simulations. (Red) Ga atoms, (Blue) Al atoms, (yellow) N atoms.

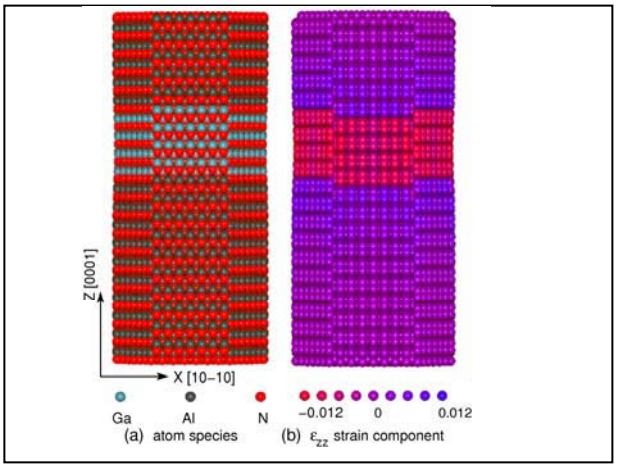

Fig. 3. Pseudomorpnically grown AlN/GaN/AlN nanowire b) Strain component ε_{zz} distribution over the nanowire.

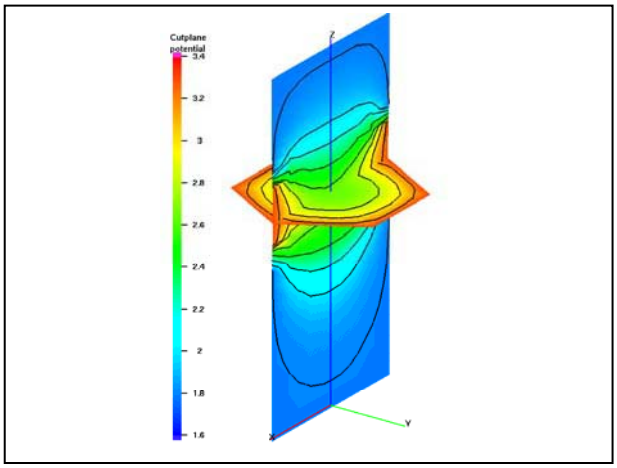

Fig. 6. Potential profile induced by the piezo and pyro polarizations in the AlGaN/GaN nanowire