Electronic properties of GaN-based quantum dot by simulations

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Simulations are performed for wurtzite GaN qauntum dot in order to investigate electronic properties which influence the optical properties eventually. The confinement potential and energies are achieved. The 6/8-band **k·p** method is used for electronic structures. Green function technique has been incorporated for 3D GaN /AlN quantum dot. Strain, piezo and pyro charges play a role related to the plane of growth in GaN crystal. The doping to the material is not used. The remaining parameters are varied in order to obtain the right structure. Quantum dots could also manifest dark exciton, a suitable candidate for qbit. Simulations make use of dispersion relations.

Keywords: Quantum dots and wires , GaN wurtzite crystal, **k·p** method, qbit.

There have been major progress and changes in the development of semiconductor quantum dots (QD) during the last decade. There has been also enhancement in QD growth technology. Self-organised and relatively uniform QD nitride structures of high quality is already shown, e.g., Stranski-Krastanow growth method. Nitride-based (wide-bandgap) quantum dots have a surpassing properties as compared to other quantum dot or quantum well structures [8] and earned a special place in optoelectronic devices. Due to its wurtzite (hexogonal) structure, which leads to strong piezoelectric and pyroelectric field in heterostructures [6]. On the other hand, the growth on the right plane, see Fig. 2, e.g., $20\bar{2}1$, can produce shorter wavelength applicable in semiconductor laser devices [2].

A GaN quantum dot embeded in AlN (GaN/AlN) is considered in detail. It has the shape of truncated hexagonal pyramid which has a height of 4 nm and a wetting layer is of 1 nm consisting of GaN. The top and the base of the the pyramid is also well defined.

One of the main feature of calculation is the simulation of strain tensor distribution in the QD in 3D, i.e., it is

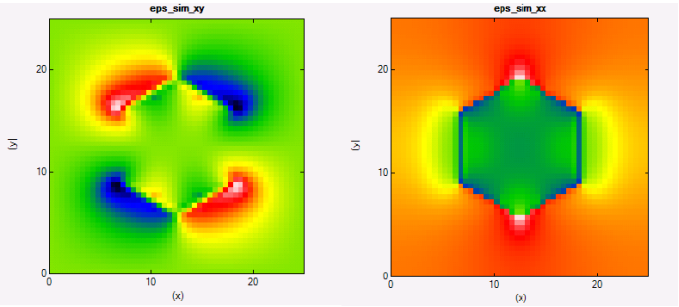

FIG. 1: Showing xy and xx component of strain tensor.

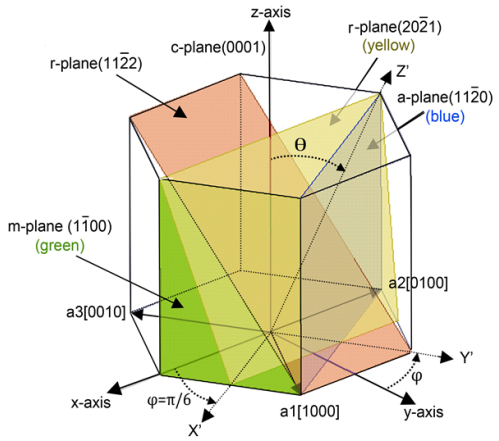

FIG. 2: Different planes are shown within wurtzite crystal.

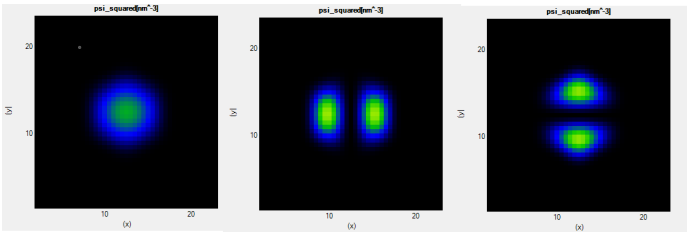

FIG. 3: Probability density distribution, $|\psi(r)|^2$, for the lowest three electron states in the GaN/AlN QD.

spacial and direction dependent, see Fig. 1. Its calculation is highly related with strain-induced piezoelectric contribution and associated with spontaneous polarization (pyroelectric charge). For this purpose a Green's function technique is used, especially suitable for zero-dimensional object like QD. Herein, the non-alignment of bands between GaN and AlN plays a big role.

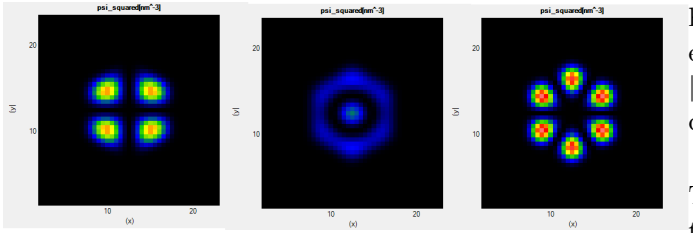

FIG. 4: Probability density distribution, $|\psi(r)|^2$, for the 4th, 5th and 6th state from the lowest electron in the GaN/AlN QD.

Probability density distributions $|\psi(r)|^2$ for the 6 lowest electron states in Ga/AlN QD are shown in Fig. 3 and Fig. 4 using 8-band **k·p**-method [1, 6] with zero spin-orbit splitting. In these figures red color shows high energy (higher $|\psi(r)|^2$) and blue color shows low energy area. Similarly, probability density distribution, $|\psi(r)|^2$, for the first six hole states in the GaN/AlN QD can be calculated.

The investigation of quantum dot and wire by simulations using Nextnano [3] remains a challenge in order to predict theoretically and be compatible with experiments. The shape of the wavefunctions calculated by Nextnano match well with other groups [4, 6]. Making use of dark-exciton as a qbit needs further innovations. It remains to be an open question [5]. This work is based on using the Nextnano software [3] and the publications as cited below [4, 6, 7]. The software has a vast variety of examples and 'input files' (commands) which could be modified for further development.

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