Theoretical study of the optical absorption spectrum in GaN/AlN quantum dots

J.M. Llorens[1] and A.García-Cristóbal
Material Science Institute, University of Valencia, P.O. Box 22085, E-46071 Valencia, Spain

III-Nitride semiconductor compounds exhibit a direct electronic band structure with energy band-gap covering the spectrum range from visible to ultraviolet. This makes them very attractive for optoelectronic device applications. However, these materials typically contain a high density of dislocations, degrading the optical efficiency of potential devices. It has been proposed that the confinement of the carriers into quantum nanostructures may dramatically reduce the scattering by the bulk defects and the rate of non-radiative recombinations. In this respect, the realization of Self-Assembled Quantum Dots (SAQDs) based on these compounds is being actively investigated [1, 2].

In this work, we perform a theoretical study of the electronic structure and optical absorption of wurtzite-type GaN/AlN SAQDs within the framework of the envelope-function approximation combined with the linear response theory. We calculate the electronic structure through the diagonalization of an 8×8 multiband $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian. The system under study presents a lattice mismatch of $\sim$ -2.4% in the basal plane. As a consequence, an inhomogeneous strain field is present in both the dot and the surrounding barrier. We have calculated this strain distribution employing a theoretical model based on the Eshelby's method of inclusions [3], as applied to hexagonal crystals by Andreev *et al.* [4]. We incorporate the effect of such strain field into our model of the electronic structure by means of the Bir-Pikus Hamiltonian. Wurtzite III-nitrides are noncentrosymmetric and uniaxial crystals. Hence, the spontaneous and strain-induced polarization results in an internal electrostatic potential which has a great impact over the electronic structure, and must be taken into account in order to construct a realistic model of the quantum dot properties. This is illustrated in Fig. 1. The left side of the figure shows a countour plot of the electrostatic potential for a truncated-cone-shaped quantum dot. The labels over the contour plot show the magnitude of the potential in eV. The dark and bright areas correspond to the regions of high and low potential, respectively.

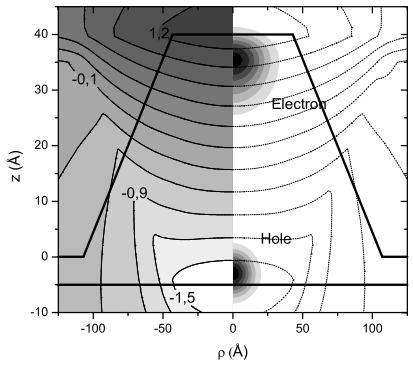

Figure 1:

[1]Corresponding author. E-mail: Jose.M.Llorens@uv.es

The inhomogeneous distribution of the potential leads to a large vertical piezoelectric field that tends to separate the electrons and holes inside the dot. This spatial separation, that can be visualized in the right side of Fig. 1, where we show the probability density distribution for the electron and hole ground states, results into a decrease of the oscillator strength and, consequently, into a reduction of the absorption (emission) intensity as compared to the case of quantum dots based on the zincblende structure.

In addition, we have calculated the exciton and biexciton states by a direct-diagonalization of the many-body Hamiltonian [5], and the corresponding absorption spectrum. We report also the dependence of the absorption on the light polarization and on the structural parameters of the system, such as quantum dot size and shape. In Fig. 2 we show how the Coulomb interaction induces a global redshift of the absorption spectra (solid line) with respect to the non-correlated case (dashed line). The binding energy of the exciton ground state Δ_x is also indicated.

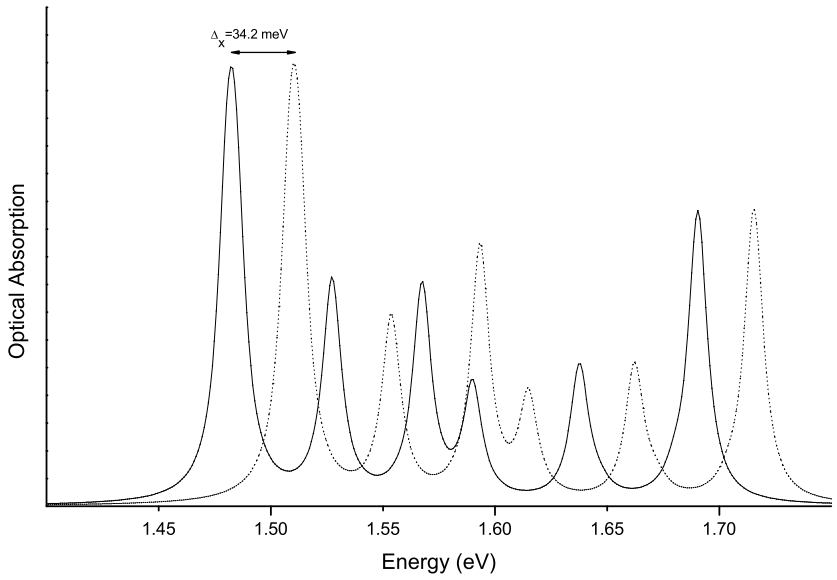

Figure 2:

References

[1] Y. Arakawa, *IEICE Trans. Electron.* **E85-C**, 37 (2002).

[2] Y.-H. Cho, B. J. Kwon, J. Barjon, J. Brault, B. Daudin, H. Mariette, and L. S. Dang, *Appl. Phys. Lett.*, **81** (2002).

[3] J. D. Eshelby, *Proc. R. Soc. London, Ser. A* **241**, 376 (1957).

[4] A. D. Andreev, and E. P. O'Reilly, *Phys. Rev. B* **62**, 15851 (2000).

[5] E. Biolatti, I. D'Amico, P. Zanardi and F. Rossi, *Phys. Rev. B*, **65**, 75306 (2002).