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Study of correlation effects on stability of many-body complexes in III–V nitride quantum dots

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Abstract

The aim of this work is to analyze theoretically the correlation energies, for neutral, positive and negative excitons and bi-excitons in the III–V nitride $In_xGa_{1-x}N/GaN$ quantum dot; where $x = 17.5\%$ denotes the indium concentration. So, we propose a model consistent with experimental observations that is small $In_xGa_{1-x}N$ truncated pyramids with circular base lying on wetting layer, both buried into GaN matrix. The correlation energies of many-body complexes X, X^-, X^+ and XX are investigated as a function of the quantum dot radius r_c and the intrinsic electric field.

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1. Introduction

III–V nitride semiconductors have been investigated very extensively in the last decade. GaN is a direct and wide band-gap semiconductor and when alloyed with InN and AlN, a spectrum from visible to ultraviolet can be covered [1,2]. These compounds are strongly polar crystals when compared to other III–V semiconductors, and thus show a piezoelectric effect [3]. Macroscopic polarization, both in intrinsic and piezoelectric nature, is unusually strong in III–V nitride, and the built in electric fields in the layers of nitride-based nanostructures, stemming from polarization change at heterointerfaces. Our main goal is to provide realistic estimation for the correlation energies of excitonic complexes while retaining at the same time a transparent formalism, which could easily be transposed to structures of actual interest, essentially for $In_xGa_{1-x}N/GaN$ in which we are interested in this work, with $x = 17.5\%$ [4].

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2. Formalism

In our calculations, quantum dots (QDs), which consist of small truncated pyramids with a circular base, are modeled by cones of height h and basis radius r_c as they are presented in Fig. 1. These pyramids have the same height h in the z growth direction and the same radius r_c in the ρ direction. The base angle of the cone is close to 30°. Seeing that the QDs diameter is as important as their height h, in addition to the internal electric field-induced quantification of energy levels of the electron and hole which takes place essentially along the z-axis. Taking into account these considerations, the QDs height is assimilated to the quantum well width. We have calculated, independently, the electron and heavy hole energy levels, neglecting light hole effect, excitonic effects and spin–orbit effect. Due to cylindrical symmetry of the system, the problem is 2D and the QDs confinement-potential couples the motion along growth direction z and radial coordinate ρ.

In this work, we use one band effective mass Hamiltonian to describe the electron and hole kinematics. The effective mass is slightly anisotropic in the conduction band: $m_{e\rho}=0.166m_0$ and $m_{ez}=0.184m_0$, and anisotropic in the valence band: $m_{h\rho}=0.504m_0$ and $m_{hz}=1.199m_0$; where m_0 is the free electron mass [4]. The confinement potential is taken as zero inside the QDs and $V_{e(h)}$ in the intermediate region between the cone and a large cylinder ($R=40$ nm and height $Z=30$ nm): $V_e=0.436$ eV and $V_h=0.187$ eV [4]. The parameters used for our calculations are given for $T=300$ K [4]. We use the matrix method [5,6] for diagonalzing the Hamiltonian over the eigenstates basis of the large cylinder leading to the electron and hole energy levels. The given wave functions are displayed on the basis of the eigenfunctions of the Schrödinger equation of a free particle in the large cylinder. The Hamiltonian of the system includes, through the electrostatic term, the effect of the static intrinsic electric fields F_a and F_b inside and outside the QDs, respectively. These fields are proportional to h, opposite, of the order of Megavolt per centimeter and oriented in the growth direction which corresponds to z [4].

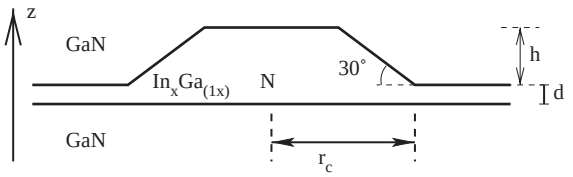

Fig. 1. Model of the QD observed in z growth direction [4].

We are interested in the correlation energy of the many-body complexes. We have to study how the static electric fields and r_c affect the correlation energies of the excitonic complexes. The coulombic interactions V_{coul}, including all possible correlations between the electrons and holes forming the excitonic complex, are evaluated at the second order of perturbation theory. The correlation energy is given by

$$\varepsilon_C = \langle f | V_{coul} | f \rangle + \sum_i \frac{|\langle e_i | V_{coul} | f \rangle|^2}{\varepsilon_f - \varepsilon_{e_i}}, \qquad (2.1)$$

where $|f\rangle$ is the fundamental state of the excitonic complex with the energy ε_f and $|e_i\rangle$ indicates the different excited states of energy ε_{e_i}. To calculate correlation energy of the bi-exciton, we assume that it is the association of positively and negatively charged excitons and then the correlation energy is obtained by adding the corresponding charged excitons as follows: $\varepsilon^{XX}_{correl} = \varepsilon^{X^+}_{correl} + \varepsilon^{X^-}_{correl}$.

3. Results

The evolution of correlation energies as a function of r_c is plotted in Fig. 2. Variations of these energies as a function of the electric fields are reported in Fig. 3. We note that for the neutral exciton, with varying r_c or the electric fields, the negative sign of correlation energies indicates that the recombination line of the exciton will take place at a lower energy than in other cases. The complex is bound in the dot. Note that for small values of r_c, the electron and hole are more localised: the exciton correlation energy is little affected by r_c variation. The other excitonic complexes are not in bound states in the QDs for all the considered values of r_c. We remark that the bi-exciton energy is the higher one. In fact, the giant internal electric field prevent the bi-exciton

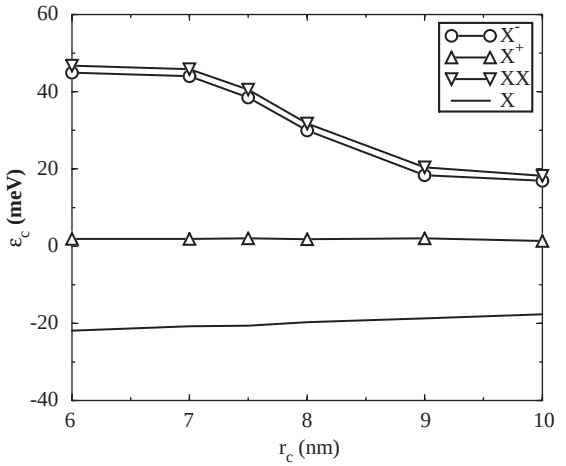

Fig. 2. Correlation energies of excitonic complexes as a function of r_c given for $F_a = 2.4$ MV/cm. The given value of the electric field F_a corresponds to $h = 3$ nm.

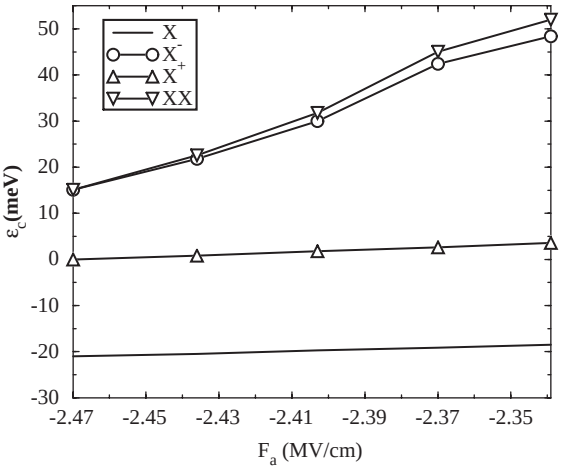

Fig. 3. Correlation energies of excitonic complexes as a function of electric field F_a ($r_c = 8$ nm).

formation in III–V nitride compounds. The evolution of exciton correlation energy as a function of the intrinsic electric field for $r_c = 8$ nm is meaningful, showing that the electron gets away from the hole. For all values of the electric field the charged excitons and bi-exciton complexes are not in bound states.

We show how the intrinsic electric field and r_c affect the correlation energies of excitonic complexes. For all values of r_c, the exciton is in the quasi-2D regime, where the coulombic effects are dominant compared to the electron and hole confinement energies. We also remark that correlation energy variation is not important. This is due to the giant internal electric field on a quasi-zero-dimension regime characterized by weak coulombic coupling compared to the energies of the independent particles. The stability of the excitonic complexes in the $In_xGa_{1-x}N/GaN$ nitride QDs is strongly affected by the existence of the giant intrinsic electric field in the QDs.

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