EXCITONS AND BIEXCITONS IN CYLINDRICAL NANOWIRES OF GROUP II-IV MATERIALS

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Abstract. A study of the trion and biexciton in a nanowire (NW) in the framework of the effective-mass model is presented. We consider the formation of trions and biexcitons under the action of both the lateral confinement and the localization potential. The analytical expressions for the binding energy and eigenfunctions of the trion and biexciton are obtained and expressed by means of matrix elements of the effective one-dimensional cusp-type Coulomb potentials whose parameters are determined self-consistently by employing eigenfunctions of the confined electron and hole states. Our calculations for the ZnO/ZnMgO, CdSe/ZnS and CdSe/CdS core/shell cylindrical shaped NWs show that the trion and biexciton binding energy in NWs are size-dependent and for the same input parameters the biexciton binding energyin NWs is always larger than the binding energy of the trion. The associative ionization of biexciton antibonding states into trion bonding states that leads to the formation of trions is studied. Based on the results for size dependence of biexciton binding energy and probability associative ionization an optimal radius for optoelectronic application NW is suggested.

1. Introduction

Recent studies of one-dimensional (1D) nanostructures nanowires [1] and nanotubes [2] show trion and biexciton binding energy depend on the electron ratio and the geometric characteristics of a nanostructure. exciton complexes like trions in solid state physics are very the few-body bound systems in atomic and nuclear physics major difference related to band effects, which make masses of the electrons and holes smaller than the bare electron and screening effects, resulting from the host lattice, which Coulomb force much weaker than in atomic systems. we present a theoretical approach to study a trion and a biexciton in a NW in the framework of the effective-mass model. We consider the formation of trions and biexciton under the action of both the lateral confinement and the localization potential. Our approach allows us to obtain analytical expressions for the binding energy and eigenfunctions of the trion and biexciton.

2. Theoretical formalism

To solve the problem of a positive trion (two holes and one electron) and biexciton (two holes and two electrons) laterally confined in a quantum NW we adopt the Born-Oppenheimer approximation, very well known in physics of molecules. The Born-Oppenheimer approximation accounts for a difference in masses of light and heavy particles and assumes that the light particles can respond almost instantly to heavy particles' displacement. The best example for a such system is a hydrogen molecular ion H_2^+ and a hydrogen molecule H_2 , which as a positively charged trion and biexciton consist from two heavy and one light and two heavy and two light particles, respectively. Therefore, instead of solving the three-body Schrödinger equation for all particle simultaneously one can treat heavy particles as motionless and solve the Schrödinger equation for a definite position of heavy particles, taking the interparticle separation as a parameter R [3]. After that calculations are carried out for different R. The application of the Born-Oppenheimer approximation naturally separates the calculation into the following steps: due to the strong lateral confinement perpendicular to the NW one first calculates the two dimensional (2D) energies and wave functions of the electron and hole, while neglecting the Coulomb interaction between them. Therefore, the fast transverse motions of charge carriers remain independent of each other. Next, using these wave functions of transverse electron and hole motion, one can average the three-dimensional (3D)Coulomb potential to a 1D Coulomb interaction between the charge carriers along the NW. Finally, after an appropriate modeling of these potentials by functions which depend on the distance between the charge carriers, one should find energies and wavefunctions for a trion or a biexciton for each fixed position of the holes by solving the corresponding reduced 1D Schrödinger equations.

3. Results

We calculate the trion and biexciton binding energies in ZnO/ ZnMgO, CdSe/ZnS and CdSe/CdS core/shell quantum structures of a cylindrical shape and study the dependence of their binding energies on the radius of the NW. Biexciton binding energy in such NWs is size-dependent. In Fig.1 we present the calculated

biexcitons's bounding energy dependence on NW's core radius (a) and shell thickness (b) for ZnO/ZnMgO and CdSe/ZnS core/shell cylindrical shaped NWs, which are prime examples for group II –IV materials. It was revealed that a radius reduction down to 1.5 nm enhances binding energy of the exciton, trion and biexciton in ZnO/ZnMgO NW, while for the biexciton in CdSe/CdS quantum NW the maximum binding energy is obtained for the thinner NW with 1 nm radius. The excitonic complexes remain stable in CdSe/ ZnS NW with the increase of the dielectric shell, while in ZnO/ZnMgO NW the trion and biexciton become unstable when the surrounding dielectric shell exceeds 2-2.5 nm.

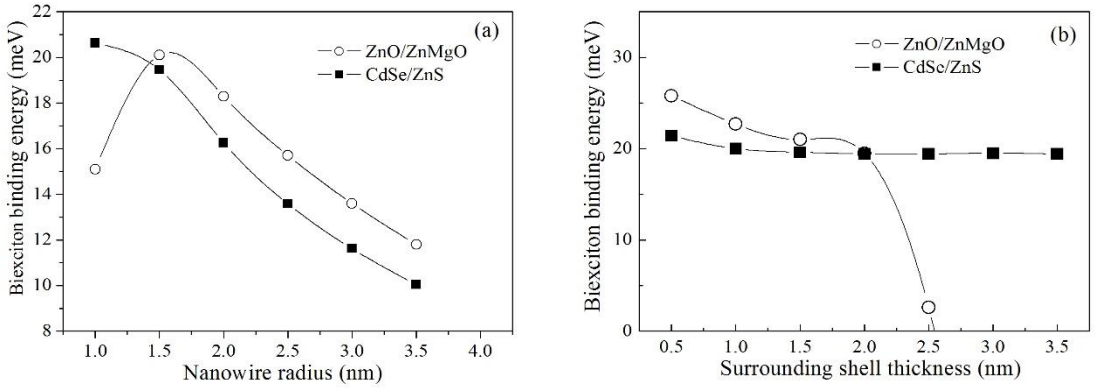

Fig.1. Dependence of the biexciton binding energy (a) on NW's core radius when shell thickness is 2 nm and (b) on the thickness of the surrounding dielectric shell when core radius is 1.5 nm.

Conclusions:

Based on the results for size-dependence of biexciton binding energy and probability associative ionization optimal radii of NWs for optoelectronic application are suggested. We suggest the mechanism of formation of the trion via associative ionization of a biexciton. As for probability of the associative ionization of biexciton into vulnerable to Auger decay trion states, it continually decreases with increasing the radius of NW. This leads us to the conclusion that 1–2 nm radius of NW should be optimal for optoelectronic application at high excitation intensity.

References:

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