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# The linear and nonlinear optical properties of an off-center hydrogenic donor impurity in nanowire superlattices: Comparison between arrays of spherical and cylindrical quantum dots



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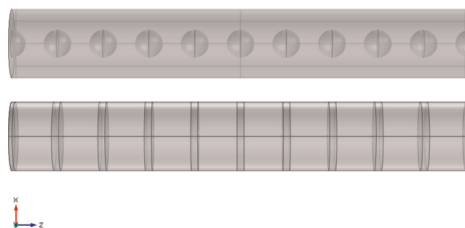
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## HIGHLIGHTS

- An off-center hydrogenic donor impurity is considered in a Sph NWSL or a Cyl NWSL.
- ACs and RI changes of Cyl NWSL are larger than those of Sph NWSL.
- Both blue and red shifts are appeared as the impurity is shifted away from the center.
- An oscillatory behavior is observed in ACs as impurity is shifted away from the center.
- Critical incident intensity depends on impurity position, Al concentration and type of NWSL.

## GRAPHICAL ABSTRACT

In this paper the effects of off-center donor impurity, Al concentration, incident intensity and relaxation time on absorption coefficients and refractive index changes of two different types of nanowire superlattices have been calculated.



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## ABSTRACT

Nanowire superlattices (NWSLs) are objects with a wide range of potential applications in nanoscale electronics and optics. In this paper, we consider an off-center hydrogenic donor impurity in two different NWSL with cylindrical cross-section which involved an array of spherical or cylindrical quantum dots (QDs) along their axis and called Sph and Cyl NWSLs, respectively. The electronic eigenstates and energy eigenvalues of NWSLs are determined by applying finite difference method. Additionally, optical properties such as linear, nonlinear and total intersubband absorption coefficients (ACs) and refractive index (RI) changes are investigated by means of compact density matrix approach. The results show that (I) optical ACs and RI changes of a Sph NWSL are smaller than those of Cyl NWSL. (II) The amplitudes of ACs and RI changes are strongly affected by impurity position and show an oscillatory behavior as the impurity shifts away from the center. (III) Resonance condition in optical spectrum can be adjusted by shape of QDs and impurity position and both blue and red shifts are appeared in ACs as the impurity shifts away from the center of NWSLs. (IV) Total optical absorption saturation intensity can be controlled by the shape of QDs or the impurity position. Moreover, optical incident intensities correspond to the saturation in optical spectrum in Cyl NWSL are smaller than their values for Sph NWSL and have a minimum values as the impurity is located at the center of barriers for both Sph and Cyl NWSLs. (V) By increasing the relaxation time the amplitude of the total AC will increase and for large values of relaxation time a saturation appears in optical spectrum which strongly depends on the Al concentration, impurity position and type of NWSL.

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## 1. Introduction

Recent advances in fabrication of semiconductor nanostructures have generated many zero-dimensional systems such as single quantum dot (QD) as an artificial atom [1], double or triple QDs as artificial molecules [2,3] and single or multilayer nanowires [4,5]. Researchers' reports reveal that nanowire structures can be formed in controlled manner [6] and have the immense potential in the different fields [7]. On the other hands, QD structure provides three-dimensional electrical confinement of the carriers [8] and the optical confinement obtained in the dot structure is smaller [9].

Semiconducting nanowires have attracted a lot of interest in the past few years due to they provide new insights into the physics of one-dimensional systems. The one-dimensional geometry of the nanowire can be taken into account as an active rejoin. Recently, one of the best applications of this active region is to utilize as host residence for a single QD [10,11] or an array of QDs which is called as a nanowire superlattice (NWSL) [12,13]. Among the various nanoscale heterostructures, the NWSLs have attracted great interest. The structure has been studied intensively in theory, experiment and computation [14–16]. The successful experimental developments of NWSLs have received increasing theoretical attention. For instance Zhang et al. [17] investigated the dynamics of a finite NWSL driven by an electric field; Niquet [18] computed the electronic structure and optical properties of InAs/GaAs NWSL; Willatzen et al. [19] calculated the magnetic field and strain effects on electronic properties of NWSL and Garcia et al. [20] investigated the effect of donor positions inside the cylindrical GaAs/GaAlAs NWSL on their ground state energies.

Moreover, the ground and excited state spectrum is of basic physical interest and is crucial for designing photoelectric devices. One of the main research topics in the area of optoelectronic deals with the intersubband optical transitions between the quantized energy levels [21]. Due to the generally larger values of transition dipole elements, in the case of intense optical intensities, nonlinear optical processes in the nanostructures are not negligible [22–24]. Meanwhile, the dependence of the optical transition energy on the confinement strength, shape and type of nanostructures make it possible to adjust the resonance conditions [25]. Therefore, because of the possibility for novel devices, the optical properties of the low dimensional semiconductor structures, including oscillator strength, linear and third order nonlinear absorption coefficient (AC) and refractive index (RI) changes have

been investigated extensively by many authors, both theoretically and experimentally [26–28].

In this paper, we focus on numerical simulation of electronic and optical properties of NWSLs with consideration of an off-center hydrogenic donor impurity. The key peculiarity of QDs is related to the 3D confinement of charge carrier and their discrete energy levels determined by QD size and shape. Therefore, in this work, we consider two different types of NWSLs: (I) an array of spherical QDs which are placed along the axis of a cylindrical nanowire and (II) a NWSL which involved an array of cylindrical QDs with the same volume of spherical QDs; which are called Sph and Cyl NWSLs, respectively. The linear, third order nonlinear and total optical ACs and RI changes of Sph and Cyl NWSLs as well as oscillator strength are calculated for both Sph and Cyl NWSLs. The paper is organized as follows. In Section 2 we introduce the model and present the theory. In Section 3 we present the numerical results. A summary is given in Section 4.

## 2. Theory

The emission and absorption of light in a semiconductor quantum structure is mediated by transitions between available electron energy levels in the material. Therefore, in first step it is necessary to calculate energy eigenvalues and corresponding wave functions of the system. We consider a cylindrical GaAs/Ga<sub>1-x</sub>Al<sub>x</sub>As nanowire superlattice (NWSL) with radius  $R_2 = 7.5$  nm and height  $l = 200$  nm. The Sph NWSL involves an array of spherical QDs with radius  $R_1$ . In fact the Sph NWSL involves  $n$  identical spherical GaAs QD, two semispherical QD at the extreme of NWSL and  $n+1$  Ga<sub>1-x</sub>Al<sub>x</sub>As barriers. The Cyl NWSL is also considered in this paper which, as mentioned, involves cylindrical QDs. A schematic view of the Sph and Cyl NWSL is presented in Fig. 1.

In the effective mass approximation and in cylindrical coordinates, the Hamiltonian of an off-center hydrogenic donor impurity can be expressed as

$$H(\rho, \phi, z) = -\frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \right) + V(\rho, z) - \frac{e^2}{4\pi\epsilon_r \epsilon_0 \sqrt{\rho^2 + (z - Z_0)^2}} \quad (1)$$

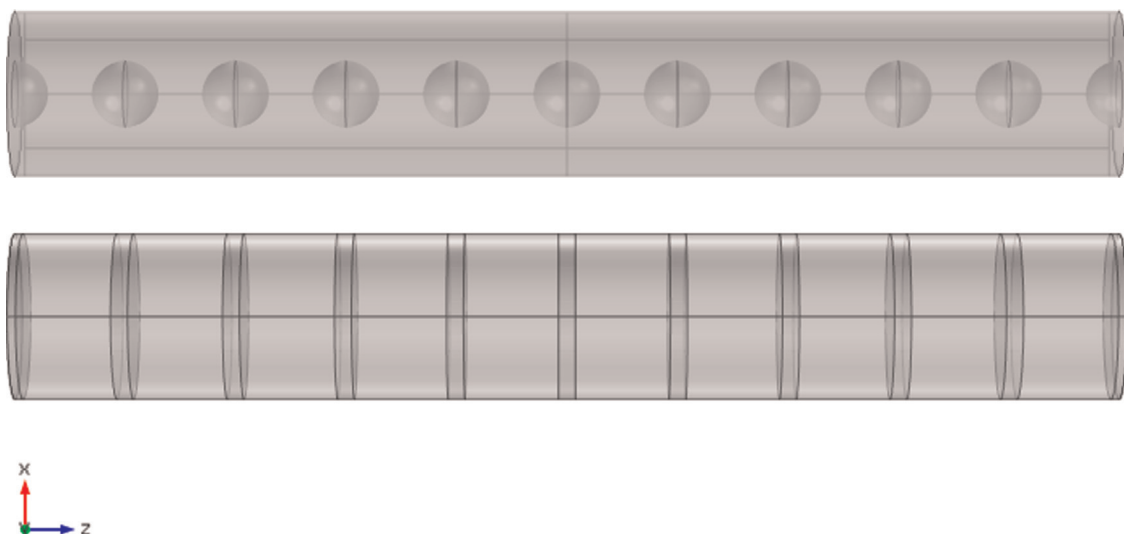


Fig. 1. A schematic view of Sph and Cyl NWSLs.

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