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Partial spin polarization of a conductance in a bi-layer $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ heterostructure based nanowire for the rectangular and the smooth lateral confinement potentials

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HIGHLIGHTS

- Spin polarization of conductance for InAlAs/InGaAs bi-layer wire is considered.
- Edge channels are formed in each layer for cleaved-edge lateral confinement.
- Substantial modifications in magnetosubbands if edge-channels are formed.
- Conductance's spin polarization limited to 40% due to edge channels
- Slight modifications of magnetosubbands' shapes for smooth lateral confinement.

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ABSTRACT

We simulate the electron transport in a vertical bi-layer nanowire in order to study an influence of the lateral confinement's shape on a spin polarization of wire's conductance. The active part of considered quantum wire constitutes a double inverted heterojunction $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ which nanostructure can be fabricated in molecular beam epitaxy process while the lateral confinement potential can be finally formed by means of cleaved overgrowth or surface oxidization methods giving the desired rectangular and smooth lateral confinement. In calculations we take into account interaction between charge carriers using DFT within local spin density approximation. We show that if the magnetic field is perpendicular to the wire axis, the pseudogaps are opened in energy dispersion relation $E(k)$ what in conjunction with spin Zeeman shift of spin-up and spin-down subbands may enhance the spin polarization of conductance with reference to a single layer wire. For nanowire with rectangular lateral confinement potential we found that the electron density has two maximums localized at wire edges in each layers. This modificates strongly all magnetosubbands giving up to four energy minimums in lowest subband and considerably diminishes widths of pseudogaps what translates into low maximal spin polarization of conductance, not exceeding 40%. This drawback is absent in wire with smooth lateral confinement. However, in order to gain a large spin polarization simultaneous tuning of magnetic field as well as the Fermi energies in both layers of nanowire are required.

1. Introduction

Influence of magnetic field on electron transport in double-nanowire system depends on mutual orientation of magnetic field and wire axis [1–3]. In longitudinal magnetic field i.e. directed parallel to wire axis, the wave functions are compressed in direction being perpendicular to electron motion what changes the tunnel coupling between layers [1,4]. On the other hand, perpendicular magnetic field may mix vertical or lateral modes leading to subbands hybridization [5,6]. Due to magnetic mixing of wave functions localized in different layers, crossings of subbands in energy dispersion relation $E(k)$ are replaced by avoided crossings. In such case, the pseudogaps are open in energy spectrum what brings severe consequences for conductance depending on quality of nanowire [5,7,8]. If transport layers are vertically stacked in nanowire, one over another, and, tilted magnetic field is applied to a system, then more pseudogaps may appear in energy spectrum since both inter-layer and intra-layer modes mixing are allowed what makes such mixing to be more effective [8]. Recently we have indicated [8] that spin polarization of conductance in bi-layer nanowire may reach up to 60% for moderate Fermi energy

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when only a few transport channels are open. Those preliminary calculations however have not taken into account an electrostatic interaction between electrons in nanosystem which may have a great impact on electron transport [9–13] and only rectangular shape of lateral confinement was considered.

In this work, we continue our theoretical studies of single electron transport in bi-layer nanowire but now we will mainly focus on spin-polarization of conductance when strong magnetic field is applied perpendicular to wire axis and electrostatic interactions between electrons are taken into account within local spin density approximation. In our considerations we model two types of lateral confinement potentials, that is, the lateral barriers will have the rectangular or smooth shapes. First type of confinement can be formed by etching of quantum wire from two-dimensional nanostructure that holds an electron gas confined within two layers and next cleaving its side surfaces. This process [14] removes defects from surfaces and then, after deposition of barrier material on both sides of nanowire gives finally side barriers without surface charge. Cross section of confinement potential of such nanowire resembles rectangular well [14]. Second type of the confinement can be formed by surface oxidization of the nanostructure. Two parallel nanogrooves created during this process may sink up to the depth of 85 nm [15] with the width of 50 nm [16]. Charge gathered on walls of each nanogrooves forms electrostatic barriers which smoothly deplete electron gas confined in both the upper and lower wells in wire. This technique is fast and very flexible since it allows for formation of much more complicated patterns of confinement potentials like e.g. laterally coupled two quantum rings [17] or a ring capacitively coupled with quantum point contact [18,19]. The shape of lateral confinement in nanowire remarkably influence on spatial distribution of electron density in quantum wire and the overall electrostatics in nanosystem. Thus, it has a strong impact on single electron transport properties [20,21].

We found that two edge wells are formed within each layer of nanowire when its lateral confinement has rectangular shape what is the result of Coulomb repulsion between electrons which push each other to opposite edge to minimize their interaction energy. An electron density localizes then in the edge wells and develops two distinct, spatially separated maximums in both layers like for two, laterally aligned and weakly coupled wires, what eventually modificates considerably the shapes of magnetosubbands. For that reason, the widths of pseudogaps are substantially reduced and the spin polarization of conductance does not exceed 40%, provided that the width of nanowire equals few tens of nanometers. However, for smooth lateral confinement we found, the electron density has only a single flat maximum in each layer what in consequence gives much less perturbed the energy dispersion relation $E(k)$ than for the rectangular confinement case and therefore makes the neighbouring magnetosubbands to be well separated on energy scale. The results of our simulations show that an accidental overlapping of spin-up and spin-down energy branches decreases the maximal value of spin polarization of conductance in a nanowire with smooth lateral confinement. Since the shapes of magnetosubbands in $E(k)$ spectrum and their splittings on energy scale depend on, besides the lateral confinement shape, also on the strength of the magnetic field and the Fermi energy, the last two quantities shall be simultaneously tuned if the value of spin polarization of conductance larger than 40% would be needed.

Paper is organized as follows. In Section 2 we will present details of theoretical model that was used in calculations, an influence of rectangular and smooth lateral confinement potentials on magnetosubbands and spin polarization of conductance of bilayer nanowire is presented and discussed in Section 3.1 and in Section 3.2, respectively. Section 4 includes conclusions.

2. Theoretical model

2.1. Model of nanostructure

The basis for fabrication of considered here two types of nanowires constitutes a two-dimensional layered lattice-matched $InP/In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ nanostructure prepared in molecular beam epitaxy process. It consists of, going from bottom to top in the growth direction, 500 nm wide buffer, δ-doping (lower) donors layer, 25 nm barrier, two 15 nm wide quantum wells separated by thin 1 nm barrier, 25 nm wide upper barrier, second δ-doping (upper) donors layer, 20 nm wide upper buffer and on the top, 10 nm wide capping layer. For simplicity, we assume that all buffers and barrier layers are made of $In_{0.52}Al_{0.48}As$, both quantum wells and top capping layer are formed within $In_{0.53}Ga_{0.47}As$ regions. The whole structure is set on n-InP substrate that is connected to bottom back gate and another, the top gate covers the surface of the nanostructure. Due to the heavily doped substrate, the back contact is ohmic [22]. However, Schottky barrier is formed at the interface InP-InAlAs and on InGaAs-top gate contact. Therefore in calculations, we have assumed that the lower buffer directly contacts with the back gate. Cross-sections of both types of bilayer nanowires are shown in Fig. 1. The height of Schottky barrier may differ much in the range 0.3–0.7 V for $In_{0.53}Ga_{0.47}As$ [23] and in the range 0.6–0.75 V for $In_{0.52}Al_{0.48}As$ [24] depending on surface roughness and material of gates. In order to remove the dependence of our results on Schottky barrier height we present them as functions of top and bottom gate voltages decreased by Schottky barrier i.e. $\Delta V_{t/b} = V_{t/b} - V_{S_{t/S_b}}$, where V_{S_t} and V_{S_b} are the

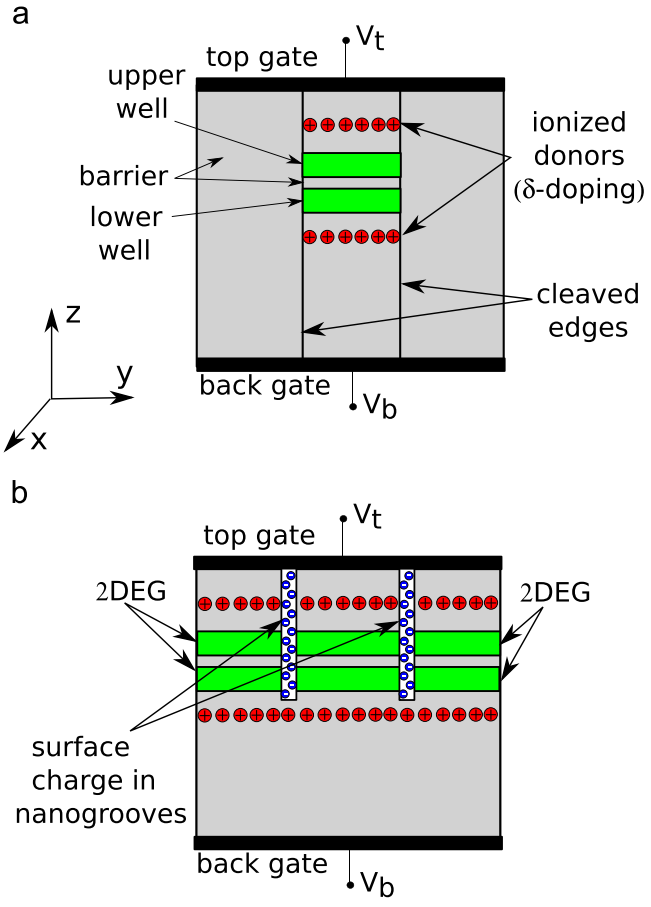

Fig. 1. Cross section of bilayer quantum wire for (a) hard wall confinement potential as can be obtained in cleaved-edge method and (b) soft lateral confinement potential due to electrons trapped on surface of the nanogrooves created with oxidization method.