



Transition from positive to negative magnetoresistance induced by a constriction in semiconductor nanowire



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HIGHLIGHTS

- Magnetotransport in InSb nanowire with a constriction is calculated.
- Change of sign of magnetoresistance as a function of the constriction radius.
- Combined effect of the geometric constriction and the spin Zeeman splitting.
- Intentionally introduced constriction may serve as a spintronic device.

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ABSTRACT

We have studied the magnetotransport through an indium antimonide (InSb) nanowire grown in [111] direction, with a geometric constriction and in an external magnetic field applied along the nanowire axis. We have found that the magnetoresistance is negative for the narrow constriction, nearly zero for the constriction of some intermediate radius, and takes on positive values for the constriction with the radius approaching that of the nanowire. For all magnitudes of the magnetic field, the radius of constriction at which the change of the magnetoresistance sign takes place has been found to be almost the same as long as other geometric parameters of the nanowire are fixed. The sign reversing of the magnetoresistance is explained as a combined effect of two factors: the influence of the constriction on the transverse states and the spin Zeeman effect.

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1. Introduction

One of the common theoretical strategies used to investigate the electronic transport in the solid state systems, and in particular in the nanostructures, is based on the calculations of the response to an external perturbation due to the electromagnetic field or temperature. Within the framework of the linear response theory, the reaction of the electron system is described by the relevant kinetic coefficients. For this reason, the studies of the magnetotransport properties of the nanowires and other nanostructures can be based on the analysis of the electron response to a suitably oriented magnetic field in terms of the magnetoresistance (MR), which is defined as the relative change of the resistance due to the applied magnetic field. The importance of this phenomenon results in the numerous practical applications, which include hard disks, memories, and various sensors.

It is worth recalling that the semiclassical theory of the

galvanomagnetic phenomena predicts the positive MR with the B^2 -dependence for the weak magnetic field B , and saturation of MR for the strong magnetic field [1–3]. A certain deviation from the semiclassical theory has been found experimentally in a number of different systems. For example, the quasi-linear B -dependence of MR is observed in the limit of the high magnetic field in the bulk n -type InSb at liquid-nitrogen temperature [4,5], and a similar dependence of MR on the magnetic field is observed in silver chalcogenides [6]. The explanation of the non-saturating properties of MR can be based on the large spatial fluctuations in the conductivity of the narrow-gap semiconductors, due to the inhomogeneous distribution of silver ions [7,8]. It has been also shown that the large positive MR is induced by the quasi-neutrality breaking of the space-charge effect in Si [9]. The large positive MR has been also reported by Schoonus et al. in boron-doped Si–SiO₂–Al structures [10].

Some of the available experimental data show that MR can be negative. In the disordered systems it can be explained by the weak localization theory, which predicts the negative MR with the \sqrt{B} -dependence [11–13]. Moreover, in the disordered systems, the

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sign of MR can be affected by the spin–orbit interaction [14–17]. Nevertheless, in organic semiconductor devices the transition between positive and negative MR due to the applied voltage and temperature has been observed [18,19], but the microscopic origin of this effect is still unclear. In Ref. [20], it has been shown that MR can be changed from positive to negative by adjusting the dissociation and charge reaction in excited states by changing the bipolar charge injection in the organic LED. A similar change of MR sign is possible in the bilayer graphene, where the gate voltage induces switching from the negative to the positive MR [21]. The mechanism responsible for the switching is related to the strong contribution from the magnetic-field modulated density of states together with the weak localization effects. Such mechanisms are also responsible for the transition from the positive to the negative MR in the double-walled carbon nanotubes [22], although Roche and Saito demonstrate that MR in such carbon nanotubes can be either positive or negative, depending on the chemical potential and the orientation of the magnetic field with respect to the nanotube axis [23]. All these examples prove that predicting the sign of MR and its field-dependence in the nanostructures is a non-trivial task.

The nanowires made of InSb are very interesting nanosystems for investigations of modern concepts in nanoelectronics, and spintronics in particular. For example, in the presence of the magnetic field, the phase coherent transport is observed in InSb nanowires at low temperatures [24]. Besides, the quantization of the conductance in the nanosystems has been experimentally confirmed more recently [25], although this quantum effect in the 3D nanowires has been predicted much earlier [26–28]. The quantization of the conductance is difficult to observe in the real nanowires due to the presence of structural and substitutional disorder, and because of the boundary roughness [25]. This stems from the fact that scattering of conduction electrons on impurities or on structural imperfections results in the change of momentum (the momentum relaxation), which leads to smearing of the step-like form of the electric conductance.

In this paper, we study the influence of the spin degree of freedom on the magnetotransport properties of the three-dimensional InSb nanowire with a constriction placed at the half-length of the nanowire, and in the presence of the magnetic field directed along the axis of the nanowire. Utilization of the MR effect in the nanowires, which can possibly replace devices of larger extents, may be seen as an opportunity to enable high sensitivity, while the small power consumption is ensured. Recent studies on nonmagnetic III–V nanowires suggest such possibility for future high-density magneto-electric devices, compatible with commercial silicon technology [29]. The available experimental reports show that the change of MR sign can be related to the applied gate voltage in a number of different materials, including organic semiconductors [18] and carbon nanotubes [22]. Electric control of MR, both its sign and magnitude, was also reported in the case of InP nanowires [30]. Our calculations show that this effect can be also induced by the presence of the constriction in the nanowire.

The paper is organized as follows. In Section 2, we present the three-dimensional model of the semiconductor nanowire with the geometric constriction, and introduce the theoretical method used to investigate the magnetotransport properties of this nanostructure in the coherent regime of the electronic transport. Section 3 contains the results of calculations and their discussion, and Section 4 – the conclusions.

2. Theory

We consider the InSb nanowire grown in [111] direction, and with a constriction in the middle of its length, as presented

schematically in Fig. 1(a). The nanowire is modeled as a cylindrical rod, which has a negligible effect on the electronic transport because we concentrate on the geometric and material parameters, for which only the ground transverse state plays a role [31].

Within the effective mass approximation, the 2×2 conduction band Hamiltonian has the form

$$\hat{\mathcal{H}} = \left[\frac{\hat{\pi}^2}{2m^*} + U_{\text{conf}}(\mathbf{r}) + eFz \right] \hat{\mathbb{1}} + \hat{\mathcal{H}}_Z + \hat{\mathcal{H}}_D + \hat{\mathcal{H}}_R. \quad (1)$$

The kinetic momentum is defined by $\hat{\pi} = \hat{\mathbf{p}} + e\mathbf{A}(\mathbf{r})$, where $\hat{\mathbf{p}}$ is the electron momentum operator, and $\mathbf{A}(\mathbf{r})$ is the vector potential, m^* is the conduction-band mass of the electron, e is the elementary charge, F is an external electric field applied along the z -axis, $U_{\text{conf}}(\mathbf{r})$ is the confinement potential energy, and $\hat{\mathbb{1}}$ is the 2×2 unit matrix. The spin Zeeman splitting term $\hat{\mathcal{H}}_Z$ is given by

$$\hat{\mathcal{H}}_Z = g^* \mu_B \mathbf{B} \cdot \hat{\sigma} \quad (2)$$

where μ_B is the Bohr magneton, g^* is the scalar electron effective Landé factor, $\hat{\sigma}$ is the vector of the Pauli matrices. For the magnetic field directed along the nanowire axis, $\mathbf{B} = (0, 0, B)$, the vector potential can be chosen in the symmetric form $\mathbf{A}(\mathbf{r}) = (\mathbf{B} \times \mathbf{r})/2$. Since the nanowire which is considered within this model is grown in the [111] direction, the Dresselhaus spin–orbit interaction is absent for momentum along the nanowire (also for the [100] nanowires, this type of the spin–orbit interaction is weak, and $\hat{\mathcal{H}}_D$ can be neglected) [32]. The last term in r.h.s. of Eq. (1) represents the Rashba interaction of the electron's spin with an electric field [33],

$$\hat{\mathcal{H}}_R = \frac{\alpha}{\hbar} \mathbf{F} \cdot (\hat{\sigma} \times \hat{\pi}). \quad (3)$$

The Rashba parameter α which measures the strength of the interaction can be given in terms of the energy band gap E_g and the spin–orbital splitting Δ_{SO} , as follows [34]:

$$\alpha = \frac{\pi e \hbar^2}{m^*} \frac{\Delta_{SO} (2E_g + \Delta_{SO})}{E_g (E_g + \Delta_{SO}) (3E_g + 2\Delta_{SO})}. \quad (4)$$

Since the electric field due to the source–drain voltage is directed along the axis of the nanowire, $\mathbf{F} = (0, 0, F)$, the Rashba Hamiltonian can be written as

$$\hat{\mathcal{H}}_R = \frac{\alpha F}{\hbar} \begin{bmatrix} 0 & \hat{\pi}_y + i\hat{\pi}_x \\ \hat{\pi}_y - i\hat{\pi}_x & 0 \end{bmatrix}, \quad (5)$$

where $\hat{\pi}_x = \hat{p}_x - eyB/2$ and $\hat{\pi}_y = \hat{p}_y + exB/2$. For the present calculations of the magnetotransport characteristics of the considered nanosystems, we assume that both ends of the nanowire are attached through the perfect contacts to the reflectionless reservoirs of electrons (source and drain). We also assume that only a small source–drain voltage is applied. Besides the fact that within the limits of the linear response theory the conductance in such case does not depend on the applied voltage, it also means that only low electric fields are present in the nanowire, and the change of the potential profile can be neglected as well as the Rashba term. However, we include in our calculations the effect of the intrinsic spin–orbit interaction which stems from the band structure by an appropriate renormalization of the electron Landé factor according to the second-order of the $\mathbf{k} \cdot \mathbf{p}$ perturbation theory [35].

The rotational symmetry of the cylindrical nanowire allows us to split $U_{\text{conf}}(\mathbf{r})$ into longitudinal $U_{\parallel}(z)$ and lateral $U_{\perp}(x, y, z)$ terms:

$$U_{\text{conf}}(x, y, z) = U_{\perp}(x, y, z) + U_{\parallel}(z). \quad (6)$$

The longitudinal confinement potential energy is determined by the position-dependent energy of the conduction-band bottom:

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