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

M. Wołoszyn,1 B.J. Spisak,1,a) P. Wójcik,1 and J. Adamowski1

AGH University of Science and Technology, Faculty of Physics
and Applied Computer Science, al. Mickiewicza 30, 30-059 Krakow, Poland

(Dated: 10 March 2016)

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.

PACS numbers: 72.20.My, 73.43.Qt, 85.75.-d, 73.63.Nm,

---
a)Electronic address: bjs@agh.edu.pl
I. 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–SiO$_2$–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 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.\textsuperscript{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,\textsuperscript{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.\textsuperscript{23} All these examples prove that predicting the sign of MR and its field-dependence in the nanostructures is a nontrivial 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.\textsuperscript{24} Besides, the quantization of the conductance in the nanosystems has been experimentally confirmed more recently,\textsuperscript{25} although this quantum effect in the 3D nanowires has been predicted much earlier.\textsuperscript{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.\textsuperscript{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.\textsuperscript{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\textsuperscript{18} and carbon nanotubes\textsuperscript{22}. Electric control of MR, both its sign and magnitude, was also reported in the case of InP nanowires.\textsuperscript{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 Sec. II, 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. Sec. III contains the results of calculations and their discussion, and Sec. IV – the conclusions.

II. 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.\textsuperscript{31}

Within the effective mass approximation, the $2 \times 2$ conduction band Hamiltonian has the form

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

The kinetic momentum is defined by $\hat{\pi} = \hat{p} + eA(\mathbf{r})$, where $\hat{p}$ is the electron momentum operator, and $A(\mathbf{r})$ 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 $\mathbf{1}$ is the $2 \times 2$ unit matrix. The spin Zeeman splitting term $\hat{H}_Z$ is given by

$$
\hat{H}_Z = g^* \mu_B \mathbf{B} \cdot \hat{\sigma},
$$

where $\mu_B$ 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 $A(\mathbf{r}) = (\mathbf{B} \times \mathbf{r})/2$. 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 $\hat{H}_D$ can be neglected).\textsuperscript{32}

The last term in r.h.s. of Eq. (1) represents the Rashba interaction of the electron’s spin
with an electric field,\(^3\)

\[ \hat{H}_R = \frac{\alpha}{\hbar} \mathbf{F} \cdot (\hat{\mathbf{\sigma}} \times \hat{\mathbf{\pi}}). \]  

The Rashba parameter \( \alpha \) which measures the strength of the interaction can be given in terms of the energy band gap \( E_g \) and the spin-orbital splitting \( \Delta_{SO} \), as follows,\(^4\)

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

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

\[ \hat{H}_R = \frac{\alpha F}{\hbar} \begin{bmatrix} 0 & \hat{\pi}_y + i\hat{\pi}_x \\ \hat{\pi}_y - i\hat{\pi}_x & 0 \end{bmatrix}, \]  

where \( \hat{\pi}_x = \hat{p}_x - e y B / 2 \) and \( \hat{\pi}_y = \hat{p}_y - e x B / 2 \). 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.\(^5\)

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,

\[ U_{\text{conf}}(x, y, z) = U_{\perp}(x, y; z) + U_{\parallel}(z). \]  

The longitudinal confinement potential energy is determined by the position-dependent energy of the conduction-band bottom: \( U_{\parallel}(z) = E_c(z) \), whereas the lateral confinement potential energy is taken in the form of the finite potential well: \( U_{\perp}(x, y; z) = U_0 \) for \( x^2(z) + y^2(z) > r^2(z) \) and \( U_{\perp}(x, y; z) = 0 \) elsewhere, where \( r(z) \) is the radius of the nanowire at the coordinate \( z \), and \( U_0 \) is the height of the potential energy barrier. In the present calculations, we assume that the radius of the constriction is given by the formula

\[ r(z) = r_0 - (r_0 - r_c) \exp \left[ - \left( \frac{z - z_0}{L_c/2} \right)^2 \right], \]
FIG. 1. (a) Schematic of the nanowire with a single constriction. $L$ is the length of the nanowire, the region of constriction has length $L_c$, and $r_0$ is the radius of the nanowire outside the constriction. (b) Dependence of the transverse eigenenergy $E_0^\perp$ on the magnetic field at two distinct $z$-coordinates, at which the radius of the nanowire is equal to 20 nm (solid lines) or 15 nm (dashed lines); $r$ is the radius of the nanowire at $z$. (c) Same as (b), but as a function of the radius of the cross-section, at $B = 0$ and $B = 6$ T.

where $L_c = 60$ nm is the length of the constriction region [cf. Fig. 1(a)], $z_0 = 100$ nm is the position of its center (measured with respect to the source, for which $z = 0$), the nanowire has length $L = 200$ nm, $r_0 = 20$ nm is the radius of the nanowire outside the constriction region, and $r_c$ is the radius of the nanowire in the middle of the constriction. Since for the values of $r_c$ less then $\sim 5$ nm the band structure strongly depends on the geometric parameters of the nanosystems,\textsuperscript{36,37} and thus the effective mass approximation is no longer valid, we limit our calculations to $r_c > 10$ nm.

One of the consequences of the dependence (7) is the formula for the energy band gap in the nanowire:\textsuperscript{38}

$$E_{g}^{nano} = E_{g}^{bulk} + aS,$$  \hspace{1cm} (8)
where $a$ is an adjustable parameter, and $S$ is the surface area to volume ratio (SVR). For the cylindrical nanowire SVR is a decreasing function of the aspect ratio parameter $2r(z)/L$. Therefore, for the geometric parameters assumed in this paper, the energy band gap in the region of the constriction changes its value by about 30% with the change of the radius for the fixed value of the bulk energy gap. This shows that the presence of the constriction in the cylindrical nanowire leads to the modification of the electronic properties, which in turn affects the spin transport.

When all the assumptions described above are taken into consideration, the Hamiltonian takes on a simplified form, and the Pauli equation can be written as

$$
\begin{bmatrix}
\hat{H}_0 + g^* \mu_B B - E & 0 \\
0 & \hat{H}_0 - g^* \mu_B B - E
\end{bmatrix}
\begin{bmatrix}
\psi_{\uparrow}(\mathbf{r}) \\
\psi_{\downarrow}(\mathbf{r})
\end{bmatrix} =
\begin{bmatrix}
0 \\
0
\end{bmatrix},
$$

(9)

where $E$ is the eigenenergy and $\psi_{\sigma}(\mathbf{r})$ is the $\sigma$ component of the spinor $[\sigma = \uparrow (\downarrow)]$. The Hamiltonian $\hat{H}_0$ has the form

$$
\hat{H}_0 = \frac{\hat{p}_z^2}{2m^*} + \frac{1}{2} \omega_c \hat{L}_z + \frac{1}{8} m^* \omega_c^2 (x^2 + y^2) + U_\perp(x, y; z) + E_c(z),
$$

(10)

with the cyclotron frequency $\omega_c = eB/m^*$, and the $z$-th component of the angular momentum operator $\hat{L}_z = x\hat{p}_y - y\hat{p}_x$. In our calculations, the energy is measured with respect to the conduction-band bottom, i.e., for the considered nanowire, which is made of homogeneous material, we put $E_c(z) = 0$.

The diagonal form of the matrix equation (9) is particularly useful for the calculations because it allows us to expand each of the spinor components in the basis of the transverse quantum states $\chi_n(x, y; z)$ for each $z$,

$$
\psi_{\sigma}(x, y, z) = \sum_n \phi_{\sigma n}(z) \chi_n(x, y; z).
$$

(11)

The coefficients $\phi_{\sigma n}(z)$ of the linear combination represent the longitudinal part of the component $\psi_{\sigma}(x, y, z)$ of the spinor. The quasi-separable form of $\psi_{\sigma}(x, y, z)$ allows us to find the transverse quantum states $\chi_n(x, y; z)$ and the corresponding transverse energies $E_n^\perp(B; z)$ by solving for each fixed $z$ the two-dimensional Schrödinger equation

$$
\hat{\mathcal{H}}_0^\perp \chi_n(x, y; z) = E_n^\perp(B; z) \chi_n(x, y; z)
$$

(12)

with the Hamiltonian $\hat{\mathcal{H}}_0^\perp$ given by

$$
\hat{\mathcal{H}}_0^\perp = \frac{\hat{p}_x^2}{2m^*} + \frac{\hat{p}_y^2}{2m^*} + \frac{1}{2} \omega_c \hat{L}_z + \frac{1}{8} m^* \omega_c^2 (x^2 + y^2) + U_\perp(x, y; z).
$$

(13)
The boundary conditions are assumed in the form \( \lim_{x,y \to \infty} \chi_n(x, y; z) = 0 \). We solve Eq. (12) by means of the variational method using the approach discussed in more detail in Ref. 31.

Since the constant value of the spin Zeeman splitting term is not appropriate for the description of spin-dependent transport phenomena in the nanosystems, an attempt to grasp this issue was made within the \( \mathbf{k} \cdot \mathbf{p} \) approach. The energy-gap dependent effective mass is given by the relation

\[
\frac{1}{m^*} = \frac{1}{m_0} + \frac{2P^2}{3\hbar^2} \left( \frac{2}{E_g} + \frac{1}{E_g + \Delta_{SO}} \right),
\]

(14)

where \( P = 9.63 \text{ eV} \cdot \text{Å} \) is the parameter of the extended Kane model, obtained for InSb from the 40-band tight-binding model by Jancu et al.\(^{40}\) For the parabolic approximation of the dispersion relation, the second order perturbation theory leads to the energy-independent expression for the effective Landé factor,\(^{39,41–43}\)

\[
g^* = g \left[ 1 + \left( 1 - \frac{m_0}{m^*} \right) \frac{\Delta_{SO}}{3E_g + 2\Delta_{SO}} \right],
\]

(15)

which depends on the band gap and the spin-orbital splitting. The symbols \( g \) and \( m_0 \) denote the Landé factor and the rest mass of the free electron in vacuum, respectively. In the present paper, the parabolic dispersion relation is assumed since we consider transport only through the lowest transverse state \( (E_{\perp}^0 < 150 \text{ mV}) \). This means that even for the relatively strong magnetic field used in our calculations (up to 8 T) we have \(|g^* \mu_B B| < 25 \text{ meV} \), and the energies of the electrons are within the range which can be well approximated by the parabolic relation.\(^{44,45}\)

For the nanostructures, Eq. (15) requires some modification to be consistent with formula (8). This problem has been addressed in Ref. 46, where the authors presented the procedure of including the quantum size effect. In line with their work, we modify the formula for the effective Landé factor of the nanowire as follows:

\[
g^*(B; z) = g \left[ 1 + \left( 1 - \frac{m_0}{m^*} \right) \frac{\Delta_{SO}}{3E_g + E_{\perp}^0(B; z) + 2\Delta_{SO}} \right].
\]

(16)

The term \( E_g + E_{\perp}^0(B; z) \), with the lowest transverse-state energy level \( E_{\perp}^0(B; z) \), can be understood as the magnetic-field and position-dependent band gap in the nanowire, \( E_{\text{g}}^{\text{nano}} \), because it depends on both the geometric parameters of the considered nanosystem and the magnetic field. The effective Landé factor calculated from formula (16) is presented in Fig. 2 for the following parameters of InSb: \( E_g = 0.235 \text{ eV}, \Delta_{SO} = 0.81 \text{ eV} \). The results exhibit interesting features that seem to be important for the \( g^* \)-factor engineering,
FIG. 2. Effective Landé factor $g^*$ as a function of the nanowire radius $r$. in the presence of the magnetic field $B = 0$, 3 T, and 6 T. Insets show $g^*$ as a function of the magnetic field $B$ calculated for the nanowire with radius $r$ equal to 10 nm, 15 nm, and 20 nm.

namely, in all the cases the effective Landé factor decreases with the increasing nanowire radius, and the limiting values of $g^*$ obtained for large radius $r$ approach the bulk values of the Landé factor for InSb. The dependence of the electron Landé factor on the magnetic field is shown in the inset of Fig. 2 for the center of the constriction (where the nanowire radius is $r = r_c = 10$ nm), and in the right inset of Fig. 2 for the region outside the constriction (i.e., for $r = r_0 = 20$ nm). The magnetic-field effect on the effective Landé factor is more pronounced outside the constriction, and in general for the nanowires with larger diameters. For a given radius, the electron Landé factor which corresponds to the lowest-energy transverse mode only weakly depends on the magnetic field $B$. This means that its value is determined mainly by the geometric parameters of the constriction, whereas the magnetic field can be regarded as a weak perturbation. The diameter-dependence of the electron Landé factor affects the spin Zeeman splitting, making it a non-linear function of the magnetic field due to the presence of the constriction. Those properties are consistent with the basic properties of the electron Landé factor which were determined within a more advanced model based on the Ogg-McCombe effective Hamiltonian that includes the non-parabolicity and anisotropy effects.47

The longitudinal part $\phi_{\sigma n}(z)$ of the spinor component $\psi_\sigma(x, y, z)$ satisfies the inhomoge-
The matrix elements $\Lambda_{nn'}(z)$ represent the coupling between the transverse modes. Since in the present calculations we assume that only the lowest-energy transverse state is occupied, we can put the right-hand side of Eq. (17) equal to zero, and solve it only for $n = 0$ to find the transmission coefficient $T_{\sigma}(E; B)$.

The magnetotransport properties of the considered nanosystem can be quantitatively characterized by the magnetoresistance (MR), which is defined as the ratio of the resistance change due to the magnetic field, $R(B) - R(0)$, to the resistance measured in zero magnetic field, $R(0)$, i.e.,

$$\text{MR}(B) = \frac{R(B) - R(0)}{R(0)}. \quad (18)$$

The resistance $R$ of the nanowire is calculated as the inverse of its conductance $G$, which is given by the sum of two spin-dependent contributions, $G = G_\uparrow + G_\downarrow$. This is a direct consequence of the Mott two-current model which is applied here. In turn, the conductance is calculated as the ratio of the spin-dependent electric current $I_{\sigma}(B)$ to the voltage $V$ applied between the ends of the nanowire, i.e., $G_{\sigma}(B) = I_{\sigma}(B)/V$. In general, the spin-dependent current can be calculated from the formula

$$I_{\sigma}(B) = e \frac{2}{h} \int_{0}^{\infty} dE \left[ T_{\sigma}(E; B)[f_{S}(E; \mu_{S}) - f_{D}(E; \mu_{D})] \right], \quad (19)$$

where $T_{\sigma}(E; B)$ is the spin-dependent transmission coefficient, and $f_{S(D)}(E; \mu_{S(D)})$ is the Fermi-Dirac distribution function for the electrons in the source $S$ (drain $D$) with the electrochemical potential $\mu_{S(D)}$. The electrochemical potentials are given by $\mu_{S} = E_{F}$ and $\mu_{D} = E_{F} - eV$, where the Fermi energy $E_{F}$ is assumed to be the same for the source and the drain. In the case of low temperature and low voltage, the conductance takes on the simple form:

$$G_{\sigma}(B) = \frac{e^2}{h} T_{\sigma}(E_{F}; B). \quad (20)$$

Finally, the total resistance of the nanowire in the presence of the magnetic field within the two-current model is given by

$$R_{\text{total}}(B) = \frac{R_{\uparrow}(B)R_{\downarrow}(B)}{R_{\uparrow}(B) + R_{\downarrow}(B)}, \quad (21)$$

where $R_{\uparrow(\downarrow)} = 1/G_{\uparrow(\downarrow)}$. Using Eqs. (18) and (21), we determine the MR of the nanowire.
III. RESULTS AND DISCUSSION

We have applied the methods presented in the previous section to determine the spin-dependent magnetotransport in the InSb nanowire with the geometric constriction in the limit of the low electric field and the low temperature. This means that we assume the coherence of the electronic transport within the linear response theory, which is sufficient for the theoretical description of the majority of transport experiments in the semiconductor nanowires in terms of the conductance.

The constriction in the nanowire creates an effective potential barrier. The additional effect due to the magnetic field is associated with the elimination of the spin degeneracy of the longitudinal electron states due to the spin Zeeman effect. It implies that the effective shape of the potential barrier created by the constriction depends on the electron spin state. In the InSb nanowire, the potential barrier for the electrons with spin up (↑) is lower than for the electrons with spin down (↓). Therefore, the transmission coefficients $T_\uparrow$ and $T_\downarrow$ are different, and the corresponding spin-dependent conductances also differ, which can be easily demonstrated using the concept of the spin conductance defined as:

$$\Delta G(B) = G_\uparrow(B) - G_\downarrow(B) .$$ (22)

Let us first investigate the influence of the constriction radius on the spin conductance in the presence of the magnetic field for the fixed radius of the nanowire ($r_0 = 20$ nm) and for the Fermi energy $E_F = 50$ meV. In this case, the coherent propagation of electrons is limited to only one transport channel, labeled by $n = 0$ in Fig. 1(b). The results presented in Fig. 3 indicate that the spin conductance $\Delta G$ is nearly zero in the two ranges of the constriction radius, in which the spin-dependent conductances in both the spin channels are almost the same: (i) in the region of the small constriction radius ($r_c < 14$ nm) $G_\uparrow \cong G_\downarrow \cong 0$, (ii) for $r_c$ near 20 nm $G_\uparrow \cong G_\downarrow \cong 1$. The non-zero values of the spin conductance correspond to $G_\uparrow \neq G_\downarrow$. In this case $G_\uparrow$ is nearly constant, while $G_\downarrow$ decreases as the magnetic field increases. This is a consequence of the increasing role of the spin Zeeman effect for the higher magnetic fields.

The above observation allows us to propose a possible application of the InSb nanowire with the constriction in spintronics. It can operate as a spin filter in which the spin filtering operation results from the joint effect of the constriction and spin Zeeman effect.
FIG. 3. Spin conductance $\Delta G$ as a function of the constriction radius $r_c$ and the magnetic field $B$ for the Fermi energy $E_F = 50$ meV.

controlled by the magnetic field. This operation is similar to the operation of the quantum point contacts.$^{53,54}$

The results of the calculations of MR based on Eqs. (18) and (21) are presented in Fig. 4. They show that the sign of MR depends on the radius of the constriction, $r_c$, and that – for each $B$ – the change of sign of MR takes place in a very narrow range, around $r_c \approx 16.8$ nm. If the radius of the constriction decreases starting from $r_c = 20$ nm, which corresponds to a nanowire without constriction, the MR gradually increases, and its sign is positive [cf. Fig. 4(b)]. The rate of change of the MR as a function of the applied magnetic field, and its maximum value together with the position of this maximum depend on the magnetic field. If the magnetic field reaches the value of 4 T, the MR is close to one, with maximum at $r_c \approx 18.5$ nm. At lower magnetic fields the maxima of MR are lower, and their position is shifted towards the smaller values of $r_c$. A further reduction of the constriction radius leads to the fairly rapid decrease of MR, which becomes negative for $r_c \lesssim 16.8$ nm. For $r_c \lesssim 15$ nm, the negative MR saturates at some constant level, which is magnetic-field dependent, e.g., the minimum of about $-0.9$ is reached for $B = 4$ T. Noteworthy, the MR calculated for spinless electrons is always non-negative [cf. dashed lines in Fig. 4(b)]. On the other hand, using suitably chosen constant value of the effective Landé factor allowed us to reproduce the change of the MR sign in the case of the geometric and material parameters used in the present calculations, and for the transport only via the lowest transverse state, but at the
FIG. 4. Magnetoresistance as a function of: (a) radius $r_c$ of the constriction and magnetic field $B$, (b) radius $r_c$ of the constriction (cross sections of (a) at different $B$; dashed lines correspond to the results obtained when spin of the electrons is neglected).

The physical interpretation of the positive/negative magnetoresistance transition (Fig. 4) can be given based on the results presented in Fig. 5. As mentioned above, the constriction in the nanowire creates the effective potential barrier for the conduction electrons, which strongly affects the transport of the electrons through the nanowire by changing the transmission coefficient. The height of this barrier at the center of the constriction, i.e., at $z = z_0$, is given by $U_\sigma(B) = E_{0z}^\perp(B; z_0) \pm g^*(B; z_0)\mu_0B$ (insets in Fig. 5).

For $B = 0$ the barrier height and the transmission coefficient are independent of the electron spin state; therefore, the only effect of the decreasing constriction radius is the increase of the potential barrier height, which causes that the transmission coefficient is reduced and the resistance increases. For $B > 0$ the spin degeneracy is lifted and the potential barrier height $U_\sigma(B)$ increases (decreases) with increasing $B$ for spin down (spin up) electrons (cf. insets of Fig. 5).

Let us consider the effect of the narrowing of the constriction on the magnetoresistance.
FIG. 5. Spin-up ($R^\uparrow$, red curves), spin-down ($R^\downarrow$, blue curves) and total ($R_{\text{total}}$, dashed lines) resistances of the nanowires for three different constriction radii $r_c$: (a) 16 nm, (b) 16.8 nm, (c) 18 nm. Insets show the effective heights of barriers at the centers of constrictions, i.e., $U_\sigma = E_{0}^\perp(B; z_0) \pm g^*(B; z_0) \mu_B B$, and $E_F$ is the Fermi energy.

For the constriction radii from the interval $17\,\text{nm} < r_c < 20\,\text{nm}$ and for either spin, $U_\sigma(B = 0) < E_F$. The spin-up barrier height $U^\uparrow(B)$ decreases with increasing $B$ [Fig. 5(c)], which causes that the transmission probability for the spin-up electrons is close to 1 and becomes independent of $B$. As a result, resistance $R^\uparrow$ is constant [cf. Fig. 5(c)]. On the other hand, potential barrier height $U^\downarrow$ increases with $B$, which reduces the transmission probability for the spin-down electrons and enlarges $R^\downarrow$. As a consequence, the total resistance increases with the increasing magnetic field [cf. Fig. 5(c)], which leads to the positive magnetoresistance for $r_c > 17\,\text{nm}$.

For $r_c = 16.8\,\text{nm}$ [Fig. 5(b)], $U_\sigma(B = 0) = E_F$. If the magnetic field increases, $U^\uparrow(B)$ and $U^\downarrow(B)$ change at approximately the same rates (but with the opposite slopes). Therefore, the growth of $R^\downarrow$ is compensated by the drop of $R^\uparrow$. As a result, the total resistance is nearly constant as a function of the magnetic field and the magnetoresistance tends to zero. The positive/negative magnetoresistance transition occurs in the very narrow interval of the constriction radii around $r_c = 16.8\,\text{nm}$ and is almost independent of the magnetic field [cf.
This feature results from the weak dependence of the total resistance on the magnetic field [Fig. 5(b)].

For $r_c < 16.8 \text{ nm}$, $U_\sigma(B = 0) > E_F$ and $U_\sigma(B)$ increases (decreases) with increasing $B$ for spin-down (spin-up) electrons [Fig. 5(a)], which leads to the increase of $R_\downarrow(B)$ and decrease of $R_\uparrow(B)$. Since the $R_\downarrow(B)$ is large for $B > 0$, according to Eq. (21), it does not affect the total resistance considerably. Then, the change of the total resistance is determined mainly by $R_\uparrow$ and decreases with increasing $B$. Therefore, the magnetoresistance is negative for the sufficiently narrow constriction [Fig. 4(b)].

**IV. CONCLUDING REMARKS**

We have studied the spin-dependent magnetotransport of the semiconductor cylindrical nanowires with the geometric constriction in the presence of the magnetic field applied parallel to the nanowire axis. The results have been obtained within the three-dimensional model of the nanowire using the adiabatic approximation, with the transverse states calculated by the variational method. The associated $z$-dependent transverse-state energies create the effective-potential barriers and modify the Landé factor, making it the position- and the magnetic-field dependent quantity. The effective $g$-factor is a monotonically decreasing function of the nanowire radius, and the effect of the magnetic field on the effective $g$-factor is negligibly small in the constriction region for the lowest-energy transverse mode. Using the two-current Mott model, we have investigated the influence of the constriction radius and the magnetic field on the spin conductance in the coherent regime of the transport. We have shown that the sign of magnetoresistance can be reverted by changing the radius of the constriction, which strongly affects the transverse states. On the contrary, the increase of the magnetic field while the radius of the constriction is kept constant leads to the increase of the magnetoresistance but does not change its sign. We have explained the positive/negative magnetoresistance transition as a combined result of the squeezing of the transverse electron states in the region of the constriction and the spin Zeeman splitting.

Finally, we want to point out that the geometric inhomogeneity, which is represented in our calculations by the single constriction, can be used as a model of either an intentionally fabricated change of the nanowire radius, or a ring-shaped gate. The present results indicate that the InSb nanowire with the constriction can operate as a spintronic nanodevice in the
coherent regime of the electronic transport, e.g., the intentionally introduced constriction can serve as a tunnel junction enhancing the spin polarization of the current flowing through the nanowire.\textsuperscript{55} The anomalous properties of the magnetoresistance, demonstrated in the present paper, can be applied in spintronics, e.g., for modifying the resistance of the spin current, or in sensor technology, e.g., for detecting the inhomogeneity of the nanowire and estimating its size.

ACKNOWLEDGMENTS

This project is supported by the National Science Centre, Poland under grant DEC-2011/03/B/ST3/00240.

REFERENCES

\textsuperscript{1}M. Dresden, Rev. Mod. Phys. \textbf{33}, 265 (1961).
\textsuperscript{2}J. M. Ziman, \textit{Electron and Phonons: The Theory of Transport Phenomena in Solids} (Oxford University Press, 2001).
\textsuperscript{3}M. I. Kaganov and V. G. Peschansky, Phys. Rep. \textbf{372}, 445 (2002).
\textsuperscript{4}H. P. R. Frederikse and W. R. Hosler, Phys. Rev. \textbf{108}, 1136 (1957).
\textsuperscript{5}J. Hu and T. F. Rosenbaum, Nature \textbf{7}, 697 (2008).
\textsuperscript{6}M. Lee, T. F. Rosenbaum, M.-L. Saboungi, and H. S. Schnyders, Phys. Rev. Lett. \textbf{88}, 066602 (2002).
\textsuperscript{7}J. Hu, M. M. Parish, and T. F. Rosenbaum, Phys. Rev. B \textbf{75}, 214203 (2007).
\textsuperscript{8}M. M. Parish and P. B. Littlewood, Science \textbf{426}, 162 (2008).
\textsuperscript{9}M. P. Delmo, S. Yamamoto, S. Kasai, T. Ono, and K. Kobayashi, Nature \textbf{457}, 1112 (2009).
\textsuperscript{10}J. J. H. M. Schoonus, F. L. Bloom, W. Wagemans, H. J. M. Swagten, and B. Koopmans, Phys. Rev. Lett. \textbf{100}, 127202 (2008).
\textsuperscript{11}A. Kawabata, J. Phys. Soc. Japan \textbf{49}, 628 (1980).
\textsuperscript{12}B. L. Altshuler, A. Aronov, A. I. Larkin, and K. D. E., Sov. Phys. JETP \textbf{54}, 411 (1981).
\textsuperscript{13}G. J. Morgan, A. Paja, and B. J. Spisak, J. Non-Cryst. Solids \textbf{270}, 269 (2000).
\textsuperscript{14}S. Hikami, A. I. Larkin, and Y. Nagaoka, \textbf{63}, 707 (1980).
15H. Fukuyama and K. Hoshino, Journal of the Physical Society of Japan 50, 2131 (1981).
16S. Chakravarty and A. Schmid, Phys. Rep. 140, 193 (1986).
17B. J. Spisak, A. Paja, and G. J. Morgan, phys. stat. sol. (b) 242, 1460 (2005).
18F. L. Bloom, W. Wagemans, M. Kemerink, and B. Koopmans, Phys. Rev. Lett. 99, 257201 (2007).
19H. Gu, J. Guo, R. Sadu, Y. Huang, N. Haldolaarachchige, D. Chen, D. P. Young, S. Wei, and Z. Guo, Appl. Phys. Lett. 102, 212403 (2013).
20J. Hu and Y. Wu, Nature 6, 985 (2007).
21Y.-F. Chen, M.-H. Bae, C. Chialvo, T. Dirks, A. Bezryadin, and N. Mason, Physica B 406, 785 (2011).
22G. Fedorov, B. Lassagne, M. Sagnes, B. Raquet, J.-M. Broto, F. Triozon, S. Roche, and E. Flahaut, Phys. Rev. Lett. 94, 066801 (2005).
23S. Roche and R. Saito, Phys. Rev. Lett. 87, 246803 (2001).
24Y. H. Yao, H. and G"unel, C. Bl"omers, K. Weis, J. Chi, J. Grace Lu, J. Liu, D. Grtzmacher, and T. Sch"apers, Appl. Phys. Lett. 101, 082103 (2012).
25I. van Weperen, S. R. Plissard, E. P. A. M. Bakkers, S. M. Frolov, and L. P. Kouwenhoven, Nano Lett. 13, 387 (2013).
26A. G. Scherbakov, E. N. Bogachek, and U. Landman, Phys. Rev. B 53, 4054 (1996).
27V. Vargiamidis and O. Valassiades, J. Appl. Phys. 92, 302 (2002).
28H. Waalkens, Phys. Rev. B 71, 035335 (2005).
29S. Li, W. Luo, J. Gu, X. Cheng, P. D. Ye, and Y. Wu, Nano Lett. 15, 8026 (2015).
30F. A. Zwanenburg, D. W. van der Mast, H. B. Heersche, L. P. Kouwenhoven, and E. P. A. M. Bakkers, Nano Lett. 9, 2704 (2009).
31M. Wołoszyn, B. J. Spisak, J. Adamowski, and P. Wójcik, J. Phys. Condens. Matter 26, 325301 (2014).
32I. van Weperen, B. Tarasinski, D. Eeltink, V. S. Pribiag, S. R. Plissard, E. P. A. M. Bakkers, L. P. Kouwenhoven, and M. Wimmer, Phys. Rev. B 91, 201413 (2015).
33S. Bandyopadhyay and M. Cahay, Introduction to Spintronics (CRC Press, 2008).
34F. G. Pikus and G. E. Pikus, Phys. Rev. B 51, 16928 (1995).
35R. Winkler, Spin–Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems (Springer, 2003).
36Y. M. Niquet, A. Lherbier, N. H. Quang, M. V. Fernández-Serra, X. Blase, and C. Delerue,
Phys. Rev. B 73, 165319 (2006).

37D. J. Carter, J. D. Gale, B. Delley, and C. Stampfl, Phys. Rev. B 77, 115349 (2008).

38D. Yao, G. Zhang, and B. Li, Nano Lett. 8, 4557 (2008).

39J. Fabian, A. Matos-Abiague, C. Ertler, P. Stano, and I. Zutic, Acta Phys. Slovaca 57, 565 (2007).

40J.-M. Jancu, R. Scholz, E. A. de Andrade e Silva, and G. C. La Rocca, Phys. Rev. B 72, 193201 (2005).

41L. M. Roth, B. Lax, and S. Zwerdling, Phys. Rev. 114, 90 (1959).

42C. Hermann and C. Weisbuch, Phys. Rev. B 15, 823 (1977).

43T. P. Smith III and F. F. Fang, Phys. Rev. B 35, 7729 (1987).

44J. R. Chelikowsky and M. L. Cohen, Phys. Rev. B 30, 4828 (1984).

45Y.-S. Kim, K. Hummer, and G. Kresse, Phys. Rev. B 80, 035203 (2009).

46A. A. Kiselev, E. L. Ivchenko, and U. Rössler, Phys. Rev. B 58, 16353 (1998).

47F. E. López, B. A. Rodriguez, E. Reyes-Gómez, and L. E. Oliveira, J. Phys. Condens. Matter 20, 175204 (2008).

48N. F. Mott, Proc. R. Soc. Lond. A 153, 699 (1936).

49M. Di Ventra, Electrical Transport in Nanoscale Systems (Cambridge University Press, 2008).

50D. Ferry, S. Goodnick, and J. Bird, Transport in Nanostructures (Cambridge University Press, 2009).

51P. Wójcik, J. Adamowski, M. Wołoszyn, and B. J. Spisak, Phys. Rev. B 86, 165318 (2012).

52P. Wójcik, J. Adamowski, M. Wołoszyn, and B. J. Spisak, Appl. Phys. Lett. 102, 242411 (2013).

53V. Bezák, Ann. Phys. 322, 2603 (2007).

54P. Wójcik, J. Adamowski, M. Wołoszyn, and B. J. Spisak, J. Appl. Phys. 118, 014302 (2015).

55E. I. Rashba, Phys. Rev. B 62, R16267 (2000).