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† In Kazan University the Electron Paramagnetic Resonance (EPR) was discovered by Zavoisky E.K. in 1944.

Spin-polarized currents in point magnetic tunnel junctions taking into account gradients of the electrochemical potential

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This work examines the conductivity properties of point contact magnetic tunnel junctions taking into account gradients of the electrochemical potentials at the ferromagnetic metal/dielectric interface. The calculations were carried out for spin-polarized currents at arbitrary ratio the point magnetic tunnel junction size and the mean free paths of conduction electrons under the applied voltage conditions. Current-voltage characteristics were obtained for symmetrical and asymmetrical point junctions.

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Keywords: Spin-polarized current, point contact, magnetic tunnel junction, magnetic heterostructure, electrochemical potential, current-voltage characteristic.

This work, dedicated to the 90th anniversary
of our (N.Kh.U. and L.R.T) Teacher,
Professor B.I. Kochelaev,
presents the latest research carried out
by the authors in the recent year

1. Introduction

Our research is devoted to the calculation of spin-polarized currents in point magnetic tunnel junctions (PMTJs) or tunnel spin valves, which have a ferromagnetic metal/dielectric (or normal metal)/ferromagnetic metal structures. These PMTJs are widely used in modern spintronic nanodevices, particularly in the field of data storage: magnetic random access memory devices, read heads of hard disk drives, programmable logic gates [1–3]. The room-temperature spin-polarized current passing through PMTJ commonly increases with increasing the bias, due to inelastic spin-flip electron scattering, inelastic electronic scattering at interface charge traps [4], as well as elastic processes involving band-structure-specific nonlinear conductance [5,6]. While much research has been carried out to study the fundamental electronic structure-related bias dependence of the electrical current in PMTJs, relatively little had been assessed on their room-temperature properties, which are important for memory applications. Moreover, investigations of spin-polarized current in PMTJ have been mostly overlooked, and little has been done from a theoretical point of view.

It is well known that PMTJ has low resistance in the case of parallel (P) alignment of magnetizations of the nanocontact sides. If their magnetizations are antiparallel (AP), then the situation can be interpreted within the framework of band theory as a mutual exchange of spin-subbands (minority or majority of electrons) in one of the magnetic domains, see Figure 1. In this case, additional resistance arises associated with the processes of electron spins interactions with magnetic moments of domain atoms. In addition, during tunnelling, the conductivity is strongly influenced by the difference in the symmetries of wave functions of tunnelling electrons in FM^L and FM^R ferromagnetic metals. The wave function of each electronic state in ferromagnetic metals has a particular symmetry, and electrons with a certain symmetry are not able to transfer directly into the states with a different symmetry [7]. Therefore, electrons at the FM^L electrode can tunnel through the barrier into the FM^R electrode only when the states specified by $k_\parallel$† in the FM^L and FM^R electrodes have the same symmetry. When FM^L and FM^R electrodes are composed of different materials, the symmetry of the wave functions of the tunnelling electrons plays an important role in tunnel conductance. In addition, the nanoscale cross-section of the intermediate layer significantly affects the conductance of PMTJ, also due to the inhomogeneity of electrochemical potentials near the interfaces [8]. In our study, we want to show the influence of the above effects by calculating spin-polarized currents as a function of the PMTJ parameters.

In our calculations, PMTJ is modeled by a circular dielectric of radius a and thickness d linking two single-domain ferromagnetic metals (FM), for example, the left FM^L and right FM^R. The z-axis of the cylindrical coordinate system is directed perpendicular to the plane of the dielectric and drawn through its center, see Figure 1. The choice of the z axis is shown for the spin conduction channel with AP alignment of magnetizations and spin up (↑).

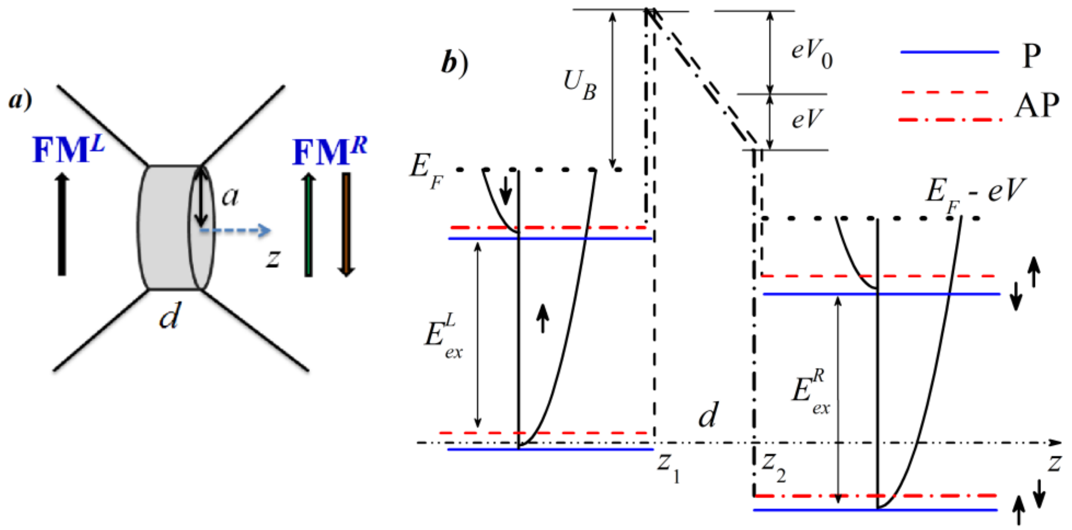

Figure 1. (Color online) **a)** Schematic representation of a PMTJ, where a is the radius and d is the thickness of the dielectric layer. The arrows show the magnetization alignment at P and AP configurations of magnetizations of the $FM^{L(R)}$ electrodes. **b)** Dispersion laws of the spin subbands of conduction electrons of two ferromagnetic metals $FM^{L(R)}$ on the left (right) side, as well as the energy potential barrier of the dielectric at an applied voltage V. V_0 is the contact potential difference between two metals. Solid lines show spin channels (↑, ↓) with P alignment of magnetizations of FM metals, dash and dash-dotted lines show spin channels (↑, ↓) with AP alignment of magnetizations. E_F is the Fermi energy level, $E_{ex}^{L(R)}$ is the exchange splitting in $FM^{L(R)}$ electrodes, U_B is the barrier height above the Fermi level.

The calculation of the spin-polarized currents was carried out within the framework of the quasiclassical theory for an arbitrary ratio of the nanocontact size (its radius and thickness) and the mean free path of conduction electrons in the FM^L and FM^R [8]. The spin-polarized current-voltage characteristics were studied as a function of the ratio of the nanocontact radius a

†The $k_\parallel$ is a projection of the Fermi wave vector on the plane of barrier. It satisfies the conservation low $k_\parallel = k_F^L \sin(\theta_L) = k_F^R \sin(\theta_R)$.

to the mean free path l of conduction electron, effective masses of electrons, and applied voltage.

2. Spin-polarized current and transmission coefficient in PMTJ

Expression for the spin-polarized current I_s (passing along the z axis through the PMTJ) was obtained based on solutions to the system of Boltzmann equations for quasiclassical Green's functions and a system of quantum mechanical equations that determine the transmission coefficients of an electron through the energy barrier taking into account the spin directions $s = (\uparrow, \downarrow)$ and applied voltage V. In the most laconic form, the expression for I_s can be written as [9, 10]

$$I_s^{\mathrm{P(AP)}} = \frac{e^2 p_{\mathrm{F},s,\min}^2\, a^2 V}{2\pi\hbar^3} \int\limits_0^\infty dk \frac{J_1^2(ka)}{k} F_s^{\mathrm{P(AP)}}(k), \tag{1}$$

where $p_{\mathrm{F},s,\min}$ is the Fermi momentum, smallest of the momenta $p_{\mathrm{F},s}^{\mathrm{L}} = \hbar k_{\mathrm{F},s}^{\mathrm{L}}$, $p_{\mathrm{F},s}^{\mathrm{R}} = \hbar k_{\mathrm{F},s}^{\mathrm{R}}$ of the contacting $\mathrm{FM}^{\mathrm{L(R)}}$; $J_1(ka)$ is the first-order Bessel function; k is the wave-number conjugate to the radial variable in the contact plane, which determines the inhomogeneity of the current density in the PMTJ. The function $F_s^{\mathrm{P(AP)}}(k)$ under integral (1) is the sum of three terms:

$$F_s^{\mathrm{P(AP)}}(k) = \left\langle \cos\theta_{c,s} D_s^{\mathrm{P(AP)}}(\cos\theta_{c,s}, d, V) \right\rangle_{c,s} + G_s^{\mathrm{heter}}(k) + G_s^{\mathrm{grad}}(k), \tag{2}$$

averaged over the solid angle of the left or right side with $c = \mathrm{L(R)}$ of the dielectric layer. Here $D_s^{\mathrm{P(AP)}}$ is the electron transmission coefficient of the tunnel barrier, $\theta_{c,s}$ is the angle between the z axis and the direction of electron motion to the interface. The other two terms, $G_s^{\mathrm{heter}}(k)$, and $G_s^{\mathrm{grad}}(k)$ are the sums of functional dependencies and integrals on the transmission coefficients D_s and parameters $k_{\mathrm{F},s}^{\mathrm{L(R)}}$, $l_s^{\mathrm{L(R)}}$, where $l_s^{\mathrm{L(R)}}$ are the spin-dependent mean free paths. The explicit form of $G_s^{\mathrm{heter}}(k)$ and $G_s^{\mathrm{grad}}(k)$ are given in article [9]. The second term $G_s^{\mathrm{heter}}(k)$ is used to calculate the spin-polarized current with a nonuniform distribution of the electron flow in the constriction of the contact. The third term $G_s^{\mathrm{grad}}(k)$ takes into account the gradients of electrochemical potentials at the boundaries of the PMTJ layers.

The conduction electron transmission coefficient through the PMTJ for one conduction spin channel and at an applied voltage $V > 0$ (the electron moves from left to right) is equal to

$$D(\cos\theta_{\mathrm{L}}, d, V) = \frac{4k_{\mathrm{L}}k_{\mathrm{R}}m_{\mathrm{L}}m_{\mathrm{B}}^2 m_{\mathrm{R}}t_{\mathrm{B}}^2\,\pi^{-2}}{(k_{\mathrm{R}}m_{\mathrm{B}}m_{\mathrm{L}}\beta - k_{\mathrm{L}}m_{\mathrm{B}}m_{\mathrm{R}}\gamma)^2 + \left(k_{\mathrm{L}}k_{\mathrm{R}}m_{\mathrm{B}}^2\alpha - m_{\mathrm{L}}m_{\mathrm{R}}\chi\right)^2}, \tag{3}$$

where the perpendicular (to the dielectric plane) components of the wave vectors have the form

$$k_{\mathrm{L}} = k_{\mathrm{F}}^{\mathrm{L}}\cos\theta_{\mathrm{L}}, \quad k_{\mathrm{F}}^{\mathrm{L}} = \sqrt{\frac{2m_{\mathrm{L}}}{\hbar^2}\left(E_{\mathrm{F}}^{\mathrm{L}} \mp \frac{1}{2}E_{\mathrm{ex}}^{\mathrm{L}}\right)}; \tag{4}$$

$$k_{\mathrm{R}} = k_{\mathrm{F}}^{\mathrm{R}}(V)\sqrt{1 - \delta_{\mathrm{LR}}^2(V)(1-\cos^2\theta_{\mathrm{L}})}, \quad k_{\mathrm{F}}^{\mathrm{R}}(V) = \sqrt{\frac{2m_{\mathrm{R}}}{\hbar^2}\left(E_{\mathrm{F}}^{\mathrm{R}} \mp \frac{1}{2}E_{\mathrm{ex}}^{\mathrm{R}} + eV\right)}. \tag{5}$$

Here $\delta_{\mathrm{LR}}(V) = k_{\mathrm{F}}^{\mathrm{L}}/k_{\mathrm{F}}^{\mathrm{R}}(V)$ is the spin-asymmetry parameter of the barrier conductance channel. Under square roots, the $-$ or $+$ sign is selected for a spin channel with spin down ($\downarrow$) or spin up ($\uparrow$). When the electron moves from right to left (i.e. when $V < 0$) in Eqs. (3-5) it is necessary to change the indices L to R and R to L.

In Eq. (3) the following notation of linear combinations of Airy functions are used:

$$\begin{aligned} \alpha &= \mathrm{Ai}(\zeta_2)\mathrm{Bi}(\zeta_1) - \mathrm{Ai}(\zeta_1)\mathrm{Bi}(\zeta_2), \\ \gamma &= t_\mathrm{B}\left(\mathrm{Ai}'(\zeta_2)\mathrm{Bi}(\zeta_1) - \mathrm{Ai}(\zeta_1)\mathrm{Bi}'(\zeta_2)\right), \\ \beta &= t_\mathrm{B}\left(\mathrm{Ai}'(\zeta_1)\mathrm{Bi}(\zeta_2) - \mathrm{Ai}(\zeta_2)\mathrm{Bi}'(\zeta_1)\right), \\ \chi &= t_\mathrm{B}^2\left(\mathrm{Ai}'(\zeta_2)\mathrm{Bi}'(\zeta_1) - \mathrm{Ai}'(\zeta_1)\mathrm{Bi}'(\zeta_2)\right), \end{aligned} \tag{6}$$

where $\mathrm{Ai}'(\zeta_{1(2)})$ and $\mathrm{Bi}'(\zeta_{1(2)})$ are the first derivatives of the Airy functions, t_B factor has the form $t_\mathrm{B} = \left(2m_\mathrm{B}eV/\hbar^2 d\right)^{1/3}$. The arguments $\zeta_{1(2)}$ of the Airy functions for our problem can be written as

$$\zeta_{1(2)} = -t_\mathrm{B}\left(z_{1(2)} + \frac{E_\mathrm{F} \pm E_\mathrm{ex}^{\mathrm{L(R)}}/2 - U_\mathrm{B}}{eV}d\right), \tag{7}$$

where E_F is the Fermi energy level which is defined as the average $E_\mathrm{F} = (E_\mathrm{F}^\mathrm{L} + E_\mathrm{F}^\mathrm{R})/2$. The physical meaning of other parameters included in Eq. (3) will be determined below.

3. Current-voltage characteristics of PMTJ

Tunneling spin-polarized currents flowing through the PMTJ are significantly different for the P and AP orientations of the magnetizations of the $\mathrm{FM^L}$ and $\mathrm{FM^R}$ layers. Figure 2 *b*) shows the current-voltage characteristics for P and AP alignment of magnetizations of the contact sides for identical ferromagnetic metals $\mathrm{FM^L}$ and $\mathrm{FM^R}$. Figure 3 shows the same for different metals. In addition, as calculations have shown, the spin-polarized components of the electric currents from electrons with spin up $I_\uparrow^{\mathrm{P(AP)}}$ are several orders of magnitude higher than the components of currents from electrons with spin down $I_\downarrow^{\mathrm{P(AP)}}$. Therefore, they are not taken into account in Figure 2. The obtained dependencies show that PMTJ can operate as a device for filtering of electrons with one spin projection (spin-diode).

Frames **a)** and **b)** of Figure 2 show the spin-polarized currents of PMTJ at the magnitude of the applied voltage $V = 0.1$ V. In the frame **a)**, $k_{\mathrm{F}\uparrow,\downarrow}^{\mathrm{L(R)}}$ are the absolute values of the Fermi wave vectors, $l_{\uparrow,\downarrow}^{\mathrm{L(R)}}$ – values of the spin-dependent mean free path. In frame **b)**, U_B is the height of the energy barrier, m_B is the effective mass of electrons in the barrier in units of free electron mass m_e.

Note that $k_{\mathrm{F}\uparrow,\downarrow}^{\mathrm{L(R)}}$ are the main parameters for calculating the spin-polarized currents, since they are associated with the energy structure of the spin-subbands of the ferromagnetic metals $\mathrm{FM^{L(R)}}$. Let us also add to this that in all calculations the effective masses $m_{\mathrm{L(R)}}$ of electrons (see Eq. (3)) in $\mathrm{FM^{L(R)}}$ were taken equal to the mass m_e of a free electron. At the same time, as shown in Figure 2*a*), the mean free path $l_{\uparrow,\downarrow}^{\mathrm{L(R)}}$ of conduction electrons for identical ferromagnetic metals $\mathrm{FM^L}$ and $\mathrm{FM^R}$ were taken to be different. We took the same values of $l_{\uparrow,\downarrow}^{\mathrm{L(R)}}$ when calculating the spin components of the current in the cases shown in Figure 3.

Curves in Figure 2*a*) show that in the case of small $a/l_\uparrow^\mathrm{L}$ ratios, corresponding to the ballistic transport of electrons through PMTJ, the dependence of $I_\uparrow^\mathrm{P}$ for the P alignment of the magnetizations of the $\mathrm{FM^{L(R)}}$ layers exceeds the $I_\uparrow^\mathrm{AP}$ for the AP alignment. The dashed blue curve is calculated taking into account gradients of electrochemical potentials, the solid curve is calculated without gradients, at P alignment of the magnetizations of the $\mathrm{FM^{L(R)}}$ electrodes. However, at AP alignment of magnetization of $\mathrm{FM^{L(R)}}$ electrodes, the dashed and solid red curves on the scale of Figures 2**a)** and 2**b)** almost coincide. In addition, we note that more careful calculations show that in the ballistic case, when $l_s^{\mathrm{L(R)}} > a$, accounting for gradients

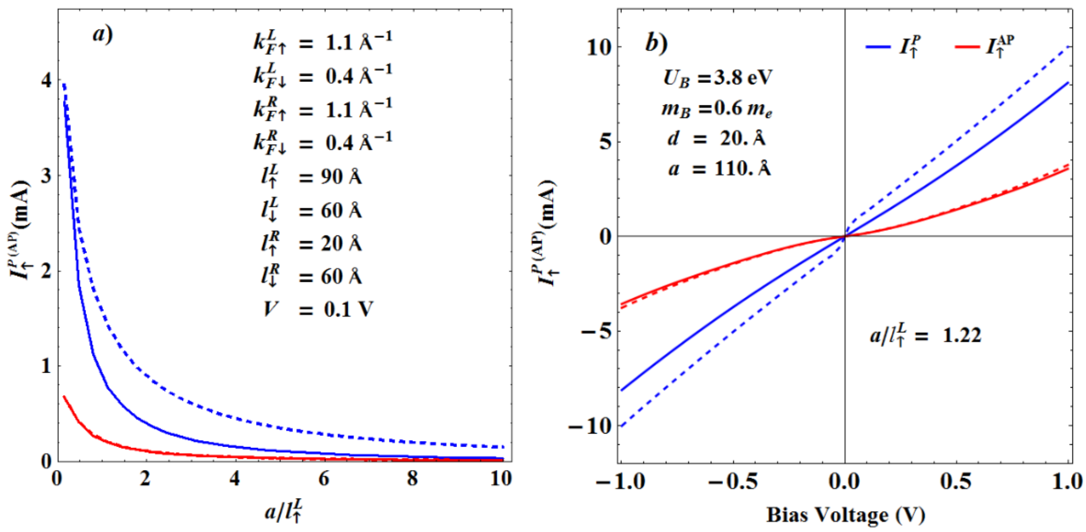

Figure 2. (Color online) Current-voltage characteristics for symmetrical PMTJ are shown. **a)** Dependences of the spin-polarized currents (with spin ↑) on the ratio of the radius a of the contact to the mean free path $l^{\mathrm{L}}_{\uparrow}$ of conduction electrons in the left $\mathrm{FM^L}$ electrode. **b)** Current-voltage characteristics (with spin ↑) of this contact obtained for $a/l^{\mathrm{L}}_{\uparrow} = 1.22$. In the graphs **a)** and **b)** the dash blue curve is calculated taking into account the gradients of electrochemical potentials, and the solid blue curve is calculated without gradients and at the P-alignment of the electrode magnetizations. The dashed and solid red curves were obtained with and without taking into account gradients at the AP alignment.

of electrochemical potentials does not lead to significant modification in the current-voltage characteristics; the dashed and solid lines coincide.

Figure 2**b)** shows the calculated current-voltage characteristics of PMTJ from spin up electrons. It can be seen that taking into account gradients of electrochemical potentials (the third term in Eq. (2)) significantly increases the current value at P alignment of magnetizations of the $\mathrm{FM^{L(R)}}$ electrodes (dashed curve). Electric current with spin up $I^{\mathrm{P(AP)}}_{\uparrow}$ increases almost linearly with increasing the bias voltage up to 1.0 V, on the other hand, the current with spin down $I^{\mathrm{P(AP)}}_{\downarrow}$ remains very low at all bias voltages. This happens due to the much less number of conduction states available in the spin-down channel compared to the spin-up channel.

Now let's consider the current-voltage characteristics of PMTJ containing different ferromagnetic electrodes to the left and right from the dielectric layer, as well as different physical parameters of these layers, see Figure 3. In this case, the main parameters for calculating the spin-polarized currents $I^{\mathrm{P(AP)}} = I^{\mathrm{P(AP)}}_{\uparrow} + I^{\mathrm{P(AP)}}_{\downarrow}$ were taken to be different, i.e. $k^{\mathrm{L}}_{\mathrm{F}\uparrow,\downarrow} \neq k^{\mathrm{R}}_{\mathrm{F}\uparrow,\downarrow}$ for $\mathrm{FM^L}$ and $\mathrm{FM^R}$ electrodes, respectively. The electron mean free path values are given in the legend of Figure 2. The dependencies shown in Figure 3**a)** were obtained for the ratio $a/l^{\mathrm{L}}_{\uparrow} = 1.22$, and the dependencies shown in Figure 3**b)** were obtained for the ratio $a/l^{\mathrm{L}}_{\uparrow} = 0.44$. Accordingly, parameters of the dielectric layer: heights of the energy barriers U_{B}, thicknesses d and radius a, are given in the legend of Figure 3.

Note that the graphs are asymmetric with respect to the polarity of the applied voltage, i.e. show a pronounced diode effect. This diode effect is associated with the asymmetry of spin-polarized currents for an asymmetric heterostructure; the left and right electrodes $\mathrm{FM^L}$ and $\mathrm{FM^R}$ of the PMTJ are different. In the case of the paramagnetic limit (i.e., when the splitting of spin conduction subbands vanishes), the levels of spin conduction subbands in the $\mathrm{FM^L}$ and $\mathrm{FM^R}$ layers have the same positions at $V = 0$, a linear current-voltage dependence

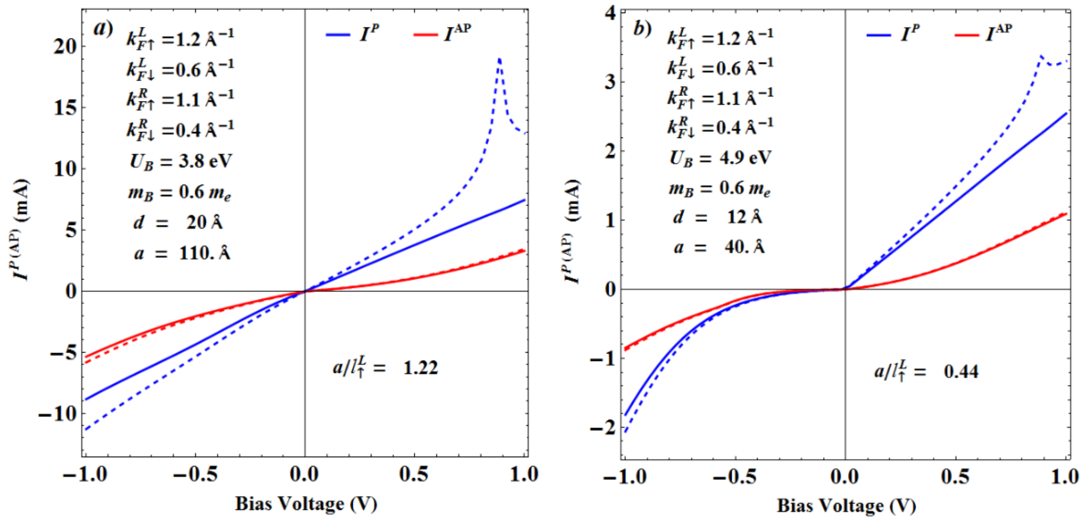

Figure 3. (Color online) Current-voltage characteristics are shown for an asymmetric PMTJ when the Fermi wave vectors $k^{\mathrm{L}}_{\mathrm{F},s}$ of the left FM^{L} electrode are different from that of the right FM^{R} electrode. **a)** The dependences were obtained for the ratio $a/l^{\mathrm{L}}_{\uparrow} = 1.22$, the remaining parameters for calculating the curves are given in the legend of Figure 2. **b)** The dependences were obtained for the ratio $a/l^{\mathrm{L}}_{\uparrow} = 0.44$, when the energy barrier height is U_{B}, radius a and thickness d of the dielectric layer are given in the legend. In both cases, the values of the mean free path of conduction electrons were taken from the legend in Figure 2. Dashed curves were calculated taking into account gradients of electrochemical potentials, solid curves are calculated without taking them into account.

is obtained. Note also that if the electrodes FM^{L} and FM^{R} have the same Fermi wave-vectors, then current-voltage characteristics similar to that in Figure 2.

In Figure 3**a)** and **b)**, the current-voltage characteristics of PMTJ, calculated taking into account gradients of electrochemical potentials (dashed curves), have unusual peaks at an applied voltage of $V \sim 0.9\,\mathrm{V}$. In our opinion, these peaks are associated with the quantization of the energy of conduction electrons near the FM/dielectric interfaces and with the narrowing of the contact area. Here the accumulation of electrons with one spin projection and its spin flip from one spin subband to another occurs. At the FM/dielectric interface, the spin-dependent electrochemical potentials μ_s have different gradients (or opposite curvatures) above and below the Fermi energy and, together with the exchange energy E_{ex}, enhance the conductivity of the electrons with one spin projection. These effects, at a certain combination of parameters of the magnetic tunnel junction with the restricted geometry, lead to the sharp increase of the spin-polarized component of the tunnel current at a certain voltage.

4. Conclusions

In this work, based on the quasiclassical theory of conduction in nano-heterostructures, the transport of electrons through point magnetic tunnel junctions is calculated. The theory covers spin-polarized quantum states of electrons, as well as ballistic and diffusion regimes of transport. Solutions include boundary conditions at the PMTJ interfaces in terms of spin-dependent gradients of electrochemical potentials and quantum-mechanical transmission coefficient.

Calculations of current-voltage characteristics show that tunnel magnetic nanoheterostructure, with certain physical and geometric parameters, can operate as an electron filtering device with one spin projection and produce a spin-diode effect in spintronics devices. This effect is associated with the mixed nature of the flow of electrons through the PMTJ, i.e., with a diffuse regime in one spin conduction channel and a ballistic regime in the other. The quasiclassical method for calculating the tunnel current $I_s^{\mathrm{P(AP)}}$ allows one to evaluate the spin-polarized current of electrons through the PMTJ in the cases of diffuse $l_s < a$ and ballistic $l_s > a$ transport. Taking into account gradients of electrochemical potentials makes it possible to approach the intermediate case, when $l_s \sim a$, and to quantitatively reproduce the experimentally observed dependence of the current on PMTJ parameters.

Acknowledgments

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