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100% spin accumulation in non-half-metallic ferromagnet–semiconductor junctions

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Abstract
We show that the spin polarization of electron density in non-magnetic degenerate semiconductors can achieve 100%. The effect of 100% spin accumulation does not require a half-metallic ferromagnetic contact and can be realized in ferromagnet–semiconductor FM–n^+–n junctions even at moderate spin selectivity of the FM–n^+ contact when the electrons with spin 'up' are extracted from n semiconductor through the heavily doped n^+ layer into the ferromagnet and the electrons with spin 'down' are accumulated near the n^+–n interface. We derived a general equation relating spin polarization of the current to that of the electron density in non-magnetic semiconductors. We found that the effect of complete spin polarization is achieved near the n^+–n interface when the concentration of the spin 'up' electrons tends to zero in this region while the diffusion current of these electrons remains finite.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The field of semiconductor electronics is based exclusively on the manipulation of charge. The phenomenal progress in increasing circuit performance by reducing device dimensions at a rate commonly referred to as that of Moore's law is likely to be curtailed by practical and fundamental limits by the next decade [1]. Consequently, there is keen interest in exploring new ideas and paradigms for future technologies. Since an electron bears spin as well as charge, combining carrier spin as a new degree of freedom with the established bandgap engineering of modern devices offers exciting opportunities for new functionality and performance. This emerging field of semiconductor physics is referred to as semiconductor spintronics [2–4]. Materials research and the physics of new spin-dependent phenomena play key roles in this rapidly growing field as researchers work to develop new magnetic materials and structures, and try to understand the basic issues of spin injection and scattering at heterointerfaces.

One may distinguish two broad regimes envisaged for spin-dependent device operation: the first in which the net spin polarization is the key parameter (i.e. there are more spins oriented in a given direction than in the opposite direction in either current or number density), and a second in which spin phase coherence is important. This article will focus on the former [5], while the latter is relevant to other avenues such as the development of spin-based quantum computation, which relies on controlled entanglement of wavefunctions [6].

One of the earliest proposals for a semiconductor spintronic device was for a spin polarized field effect transistor (spin-FET) [7], in which the source and drain contacts are ferromagnetic materials intended to inject and detect spin polarized electrons transported in a high mobility channel. The conductance of the FET would depend on electron spin orientation in the channel, which would be controlled by the gate voltage relative to the magnetization of the drain contact, producing a spin-based mode of operation. If the magnetization of the source and drain are independently controlled using techniques developed for magnetic memory, such a device offers nonvolatile and reprogrammable operation with spin or magnetization as a virtual fourth terminal. This and other device concepts, including spin-dependent resonant tunnelling diodes (spin-RTDs) [8–17], gated spin coherent devices [18, 19], spin polarized light emitting diodes (spin-LEDs) [20] and tunnel magnetoresistive devices [21–23] have stimulated tremendous interest in this rapidly growing field.

There are four essential requirements for implementing a semiconductor spintronics technology: (i) efficient electrical injection of spin polarized carriers into the semiconductor, (ii) adequate spin diffusion lengths and lifetimes for transport within the device, (iii) effective control and manipulation of the spin system, (iv) efficient detection of the spin system to determine the output. The injection of spin polarized electrons into non-magnetic semiconductors (NS) is of particular interest because of the relatively large spin coherence lifetime, τ_s, and the promise for applications in both ultrafast low power electronic devices [3, 4, 7, 24–27] and in quantum information processing (QIP) [4, 28–31].

Very encouraging progress has been made in the areas related to the manipulation and control of the spin system in non-magnetic semiconductors. Spin diffusion lengths of many microns [32, 33] and spin lifetimes >100 ns [33, 34] have been reported in optically pumped GaAs, for example. A number of successful methods have been demonstrated for manipulating and detecting [35–38] the state of the spin system. However, an efficient and practical means of electrical spin injection has heretofore been unavailable, and this lack has been a critical issue severely hampering progress in this field.

Electrical spin injection requires a contact material and a corresponding interface which facilitate the transport of spin polarized carriers into the semiconductor. Ferromagnetic metals offer most of the properties desired for a practical spin injecting contact material: a source of electrons rather than holes, high Curie temperatures, low coercive fields, and a well developed materials technology due to decades of investment largely by the recording industry. Metallization is a standard process in any semiconductor device fabrication line, so that the use of a ferromagnetic metallization could easily be incorporated into existing processing schedules.

A number of groups have attempted to inject spin polarized carriers from a ferromagnetic metal contact into a semiconductor and reported measured effects of the order of 0.1–1%, with an estimate of actual spin polarization in the semiconductor extracted from a particular model [39–41]. These experiments measured a change in resistance or potential, which some argue may be compromised by contributions from anisotropic magnetoresistance or a local Hall effect [42–44].

Recent model calculations by several groups [45–48] have indicated that the large difference in conductivity between a metal and semiconductor severely inhibits spin injection.

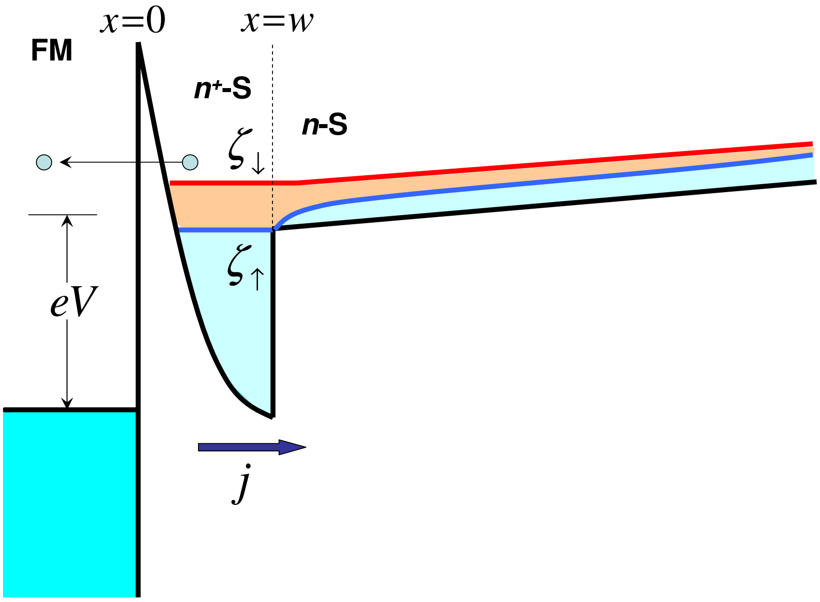

Figure 1. Schematic view of the proposed FM–n^{+}–n heterostructure designed to create 100% spin polarized non-equilibrium electron gas.

In an overly simplistic picture, the ability of the semiconductor to accept carriers is independent of spin, and much less than that of the metal to deliver them. Consequently, equal numbers of spin up and spin down electrons are injected regardless of the metal initial polarization, resulting in essentially zero spin polarization in the semiconductor. In the diffusive transport regime (where all existing devices operate), successful spin injection occurs only for two conditions: either the conductivities of the FM contact material and semiconductor are closely matched, or the contact is 100% polarized. If neither condition is satisfied, the spin polarization in the semiconductor is very low ($<1\%$). No FM metal meets either of these criteria. Half-metallic materials offer 100% spin polarization in principle [49, 50] although defects such as antisites or interface structure rapidly suppress this value [51].

It was suggested that this obstacle of conductivity mismatch could be circumvented if the interface resistance dominates, e.g. by insertion of a tunnel barrier between the metal and semiconductor [52]. The physics was first elucidated theoretically by Rashba [52], who noted that such an approach supported a difference in chemical potential between the spin up and spin down bands at the interface, thereby enabling the use of FM metals as spin injecting contacts. Various oxides are commonly used as tunnel barriers. Magnetic metal/Al_2O_3/metal structures have been extensively studied, since they form the basis for a tunnelling spectroscopy used to determine the metal spin polarization [53], and for TMR devices being developed for nonvolatile memory [22].

However, for a metal contact on a semiconductor, the band bending accompanying Schottky barrier formation provides a very natural potential barrier, as shown in figure 1. For moderately doped semiconductors ($n \sim 10^{16}$–10^{18} cm^{-3}), the depletion width is hundreds of ångströms [54] and very little electron current flows from the metal under reverse bias, characteristic of a rectifying contact. However, this width may be readily controlled by an appropriate doping profile since heavily doping the surface of the semiconductor during MBE growth reduces the depletion width to tens of ångströms [55] so that tunnelling from the metal into the semiconductor becomes a highly probable process. This approach avoids the use of a discrete barrier layer and the accompanying problems with pinholes, and Schottky contacts are already routine ingredients in semiconductor technology.

This tailored Schottky tunnel barrier approach was successfully demonstrated by Hanbicki *et al* using an epitaxial Fe film on an AlGaAs/GaAs QW spin light emitting diode (spin-LED) heterostructure [56, 57] and electron spin polarizations of 32% were achieved in the GaAs QW. The LED structures were grown using an AlGaAs contact layer doping profile designed to enhance tunnelling. Electroluminescence (EL) data from surface emitting devices were obtained and analysed as a function of magnetic field. The field was necessary to align the Fe magnetization (carrier spins) along the surface normal (Faraday geometry) so that the familiar quantum selection rules can be applied. The spectra were dominated by the QW heavy hole exciton, with a linewidth of 5 meV. At zero field, the right $\mathcal{P}_+$ and left $\mathcal{P}_-$ circularly polarized EL components were equal, as expected, since the easy magnetization axis of the Fe film lies in the plane. As the Fe magnetization was rotated out of the plane, the $\mathcal{P}_+$ component dominated and a pronounced difference in intensities was observed in the raw data, signalling successful electrical spin injection. The circular polarization directly tracks the out-of-plane magnetization of the Fe film obtained by independent magnetometry measurements. We emphasize that 32% is the spin polarization of the *number* rather than the current density, which is always the case for experiments on the optical detection of the spin injection.

The experiments by Hanbicki *et al* [56, 57] were in many respects inspired by Rashba's theory of spin injection [52], which is based on the diffusion approximation, and assumes a spin-selective tunnel contact between the FM and semiconductor. More precisely, the tunnel contact has different conductances for up and down spins and spin relaxation at the interface is neglected. The results highlight two requirements for efficient spin injection: (i) the mesoscopic contact (interface) resistance must dominate, and (ii) the contact (interface) must be spin selective. Rashba's theory is limited to the ohmic regime, while in reality large biases often lead to nonlinear current–voltage characteristics. Nevertheless, the theory provides simple and physically sound guidance on how to increase spin injection efficiencies, for example, by increasing the spin selectivity of the contact resistance.

In principle, any tunnel contact between a FM material and a non-magnetic material will be spin selective, because the spin polarization of the density of states leads to spin polarization of the tunnel current. While the density of states is not explicitly present in the Landauer formula, which is commonly used in microscopic transport calculations, it can be shown that the transmission coefficient is proportional to the product of the densities of states in the emitter and collector [58]. Therefore, one obvious way to improve spin injection is to use highly spin polarized, or even *half-metallic*, ferromagnetic emitters. Most ferromagnetic materials, however, are not half-metallic, and therefore alternative strategies are important. Moreover, if one's goal is to create a maximal spin imbalance of the electron density (spin accumulation) in a non-magnetic semiconductor, in the same way as is done in the optical pumping experiments [33, 34], the spin injection may not be the most efficient method for achieving this goal. Indeed, the spin injection is enabled by the tunnelling of the electrons from FM into NS through a spin-selective barrier. But the tunnelling is a symmetric process and, consequently, the tunnelling of the electrons from the semiconductor into the ferromagnet will also produce spin accumulation in NS. This process is called spin extraction [59–62]. In this article we will demonstrate that the spin accumulation may reach 100% when the spins are extracted from NS into FM through a specially tailored interface. Surprisingly, this complete spin extraction does not require a half-metallic FM contact and can be achieved at rather modest spin selectivities of the contact. Therefore, some other properties of the ferromagnetic contacts, such as robustness of the ferromagnetism, quality of the FM/NS interface, can be taken into consideration in designing the most efficient and stable magnetic heterostructures.

For any spin-dependent quantity, e.g. current density j_σ or number density n_σ, we will introduce their symmetric, e.g. $j = j_\uparrow + j_\downarrow$ (total current), and antisymmetric, e.g. $\Delta j = j_\uparrow - j_\downarrow$ (spin current), combinations. The main characteristics of the spin injection or spin extraction are the spin polarizations of the electron (i.e. number) density $P = (n_\uparrow - n_\downarrow)/n = \Delta n/n$ and the current density $\gamma = (j_\uparrow - j_\downarrow)/j = \Delta j/j$. The value of γ determines a magnetoresistance ratio and performance of spin-valve devices [7, 52, 47, 27, 26]. The value of P determines the polarization of the recombination radiation measured in most of the experiments on optical detection of spin injection [56, 57, 63]. Moreover, a high value of P is crucial for QIP devices [4, 29, 30]. It has been implied in most of the previous theoretical works on spin injection [64–66, 52, 47, 48, 67, 68, 61, 60] that P cannot exceed γ. This assumption is consistent with existing observations in which different magnetic materials such as magnetic semiconductors or ferromagnetic metals (FM) have been used as injectors of spins into semiconductors [3, 4].

The major effort has been concentrated on finding the means to increase the spin injection coefficient, i.e. the value of γ at an interface between a ferromagnet and a semiconductor. The main reason for this is that the spin injection coefficient defines a magnetoresistance ratio for spin-valve devices [52, 47]. Furthermore, it has been implied in previous theoretical works on spin injection [64–66, 52, 47, 48, 67, 68, 61, 60] that P cannot exceed γ. This assumption is consistent with existing observations in which different magnetic materials such as magnetic semiconductors, half-metallic ferromagnets, and ferromagnetic metals (FM) have been used as spin injectors [3, 4] in reverse-biased junctions. That is why the value of P which is measured in the experiments on optical detection of the spin injection [56, 57, 63] has been taken as a lower bound of the spin injection coefficient.

It follows from a formal consideration by Yu and Flatte [48, 67] that P can, in principle, exceed γ in non-degenerate semiconductors when electron spins are extracted from NS into FM (reverse bias). However, more detailed studies by Osipov and Bratkovsky [27, 26], taking into account tunnelling through a Schottky barrier in simple FM–NS junctions, revealed that $P < \gamma$ due to a feedback formed during the tunnelling process. The condition $P < \gamma$ holds for both non-degenerate and degenerate semiconductors and for both reverse- and forward-biased simple FM–NS junctions [60–62].

In this paper we demonstrate a possibility for achieving complete spin polarization $P \sim 1$ of electrons in *degenerate* semiconductors near forward-biased FM–S junctions with moderate spin selectivities of the FM contacts. The effect is based on spin extraction and nonlinear dependence of the non-equilibrium spin density on the electric field. A non-equilibrium electron gas becomes completely spin polarized when a quasi-Fermi level ζ_σ for one type of carrier (e.g. $\sigma = +1(\uparrow)$) reaches the bottom of the conduction band E_c near a specially tailored interface. This opens up new exciting opportunities because the work for many spintronic devices would drastically depend on (potentially high) values of P. It would be highly desirable to develop capabilities of creating a highly spin polarized electron gas with $P \sim 1$ in a channel of a field effect transistor for Datta–Das-type devices [7], and also for the purposes of quantum information processing, for quantum memories based on nuclear spin polarization, for potential devices based on the spin Hall effect, and for many other applications.

Unlike in previous works where simple FM–NS junctions were studied, in this article we consider a band-engineered FM–n^+–n structure containing a thin superheavily doped n^+ layer and a degenerate semiconductor n region (figure 1). The effect in question is based on spin extraction and nonlinear dependence of the non-equilibrium spin density on the electric field. A non-equilibrium electron gas becomes completely spin polarized when a quasi-Fermi level for one type of carrier (e.g. $\zeta_\uparrow$) reaches the bottom of the conduction band E_c near the n^+–n interface. The spin extraction from NS as predicted by Zutic *et al* [59] for forward-biased p–n junctions containing a magnetic semiconductor was studied in detail for FM–NS junctions [27, 26], and was experimentally found in forward-biased MnAs/GaAs Schottky junctions [69]. However, both the predicted and observed values of the spin polarization P were rather small.

2. Spin polarized transport in non-magnetic semiconductors

We start from a consideration of a non-magnetic semiconductor with non-equilibrium spin imbalance described by a quasi-Fermi distribution:

$$n_\sigma(x) = \int N(\varepsilon - E_c) f\left[\frac{\varepsilon - \zeta_\sigma(x) - e\varphi(x)}{kT}\right] \mathrm{d}\varepsilon. \tag{1}$$

Here $N(\varepsilon - E_c)$ is the density of states, $f(x) = (\exp(x) + 1)^{-1}$ is the Fermi function, e is the magnitude of the elementary charge, and $\phi(x)$ is the electrostatic potential. The current density j_σ can be expressed as

$$j_\sigma = e\mu n_\sigma E + eD_\sigma \frac{\partial n_\sigma}{\partial x} = \mu n_\sigma \frac{\partial \zeta_\sigma}{\partial x}. \tag{2}$$

Here $E = -\partial\varphi/\partial x$ is the electric field, $\mu = e\tau^{\mathrm{coll}}/m$ is the mobility, τ^{coll} is the collision (momentum relaxation) time, m is the effective mass and D_σ is the diffusion coefficient. The second part of equation (2) is based on the generalized Einstein relations [70]

$$\mu = eD_\sigma \frac{\partial \ln(n_\sigma)}{\partial \zeta_\sigma}, \tag{3}$$

which ensure that charge and spin currents vanish in equilibrium ($\zeta = \mathrm{const}$, $\Delta\zeta = 0$).

Le us express the spin-dependent current and number densities through their spin polarizations:

$$n_\sigma = \tfrac{1}{2} n(1 + \sigma P) \tag{4}$$

$$j_\sigma = \tfrac{1}{2} j(1 + \sigma\gamma), \tag{5}$$

where $\sigma = \pm 1$. Substituting equations (4) and (5) in equation (2) we obtain

$$\gamma = \frac{\Delta j}{j} = \frac{\partial\Delta\zeta/\partial x + P\partial\zeta/\partial x}{\partial\zeta/\partial x + P\partial\Delta\zeta/\partial x}. \tag{6}$$

Here $\zeta = \zeta_\uparrow + \zeta_\downarrow$ and $\Delta\zeta = \zeta_\uparrow - \zeta_\downarrow$.

Let us make use of the condition

$$j = j_\uparrow + j_\downarrow = \frac{\mu n}{2}(\partial\zeta/\partial x + P\partial\Delta\zeta/\partial x) = \mathrm{const}. \tag{7}$$

Using equation (2) and taking into account the steady-state condition $j = \mathrm{const}$ we can relate spin polarizations γ and P:

$$\gamma = P + (1 - P^2)\frac{\mu n}{2j}\frac{\partial\Delta\zeta}{\partial x}. \tag{8}$$

The first term in this equation can be interpreted as a spin drift term while the second one can be interpreted as a spin diffusion term. We will always assume that the FM metal is on the left-hand side and the semiconductor is on the right-hand side of the interface $x = 0$. We will also assign directions ‘up’ and ‘down’ to the majority and minority spins in the ferromagnet respectively. This convention ensures that γ is always positive and does not depend on the direction of the current. On the other hand the spin polarization of the electron density P does depend on the sign of j. Namely, under the reverse bias (spin injection—electrons are moving from FM to S) $j < 0$ and $P > 0$, i.e. the majority spins are accumulating in the semiconductor near the interface while under the forward bias (spin extraction—electrons are moving from S to FM) those are the minority spins, i.e. $j > 0$ and $P < 0$. The magnitude of the spin polarization $|P|$, however, is always decaying away from the interface.

At this point it is convenient to introduce a local electroneutrality approximation, $n = n_0$, where n_0 is the equilibrium electron density, and simplify equation (8):

$$\gamma = P + \frac{en_0 D(P)}{j}\frac{\mathrm{d}P}{\mathrm{d}x}, \tag{9}$$

where we have introduced a bi-spin diffusion coefficient:

$$D(P) = \frac{\mu}{2e}(1-P^2)\frac{\mathrm{d}\Delta\zeta(n_0, P)}{\mathrm{d}P}. \tag{10}$$

The steady-state continuity equations for spin-dependent currents in a homogeneous, non-magnetic semiconductor read

$$\begin{aligned} \frac{\mathrm{d}j_\uparrow}{\mathrm{d}x} &= \frac{e}{2\tau_s}\left(n_\uparrow - n_\downarrow\right) \\ \frac{\mathrm{d}j_\downarrow}{\mathrm{d}x} &= \frac{e}{2\tau_s}\left(n_\downarrow - n_\uparrow\right), \end{aligned} \tag{11}$$

where τ_s is a spin-flip time. Let us consider the case of a degenerate semiconductor at low temperatures. Then

$$\Delta\zeta = \frac{mv_\mathrm{F}^2}{2}\left[(1+P)^{2/3} - (1-P)^{2/3}\right], \tag{12}$$

where $v_\mathrm{F} = (\hbar/m)(3\pi^2 n_0)^{1/3}$ is the equilibrium Fermi velocity. Substituting equation (12) in equation (10) we obtain

$$D(P) = \frac{v_\mathrm{F}^2\tau_\mathrm{coll}}{3}\tilde{D}(P), \tag{13}$$

where

$$\tilde{D}(P) = \tfrac{1}{2}(1-P^2)^{2/3}\left[(1+P)^{1/3} + (1-P)^{1/3}\right]. \tag{14}$$

Now we introduce the spin diffusion length $L_s^2 = (v_\mathrm{F}^2\tau_\mathrm{coll}\tau_s)/3$ and dimensionless variables of length $\xi = x/L_s$ and current $\epsilon = j/j_s$, where $j_s = en_0 L_s/\tau_s$. In terms of these variables equations (11) and (9), read

$$\epsilon\frac{\mathrm{d}\gamma}{\mathrm{d}\xi} = P, \tag{15}$$

$$\gamma = P + \frac{\tilde{D}(P)}{\epsilon}\frac{\mathrm{d}P}{\mathrm{d}\xi}. \tag{16}$$

Substitution of equation (16) in equation (15) leads to a non-linear drift–diffusion equation:

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\tilde{D}(P)\frac{\mathrm{d}P}{\mathrm{d}\xi}\right) + \epsilon\frac{\mathrm{d}P}{\mathrm{d}\xi} - P = 0. \tag{17}$$

Instead of dealing with the second-order non-linear equation (17) we can derive a first-order equation relating γ and P:

$$\epsilon^2\frac{\mathrm{d}\gamma}{\mathrm{d}P} = \tilde{D}(P)\frac{P}{\gamma - P}. \tag{18}$$

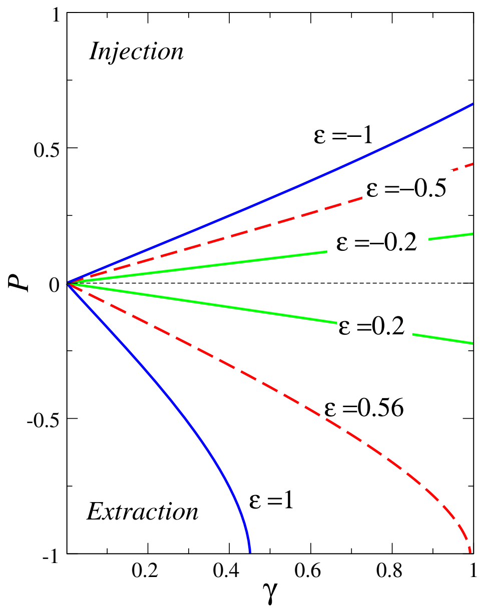

Figure 2. Solutions of equation (18) for different ϵ.

As $\xi \to \infty$, $P \to 0$ and $\mathrm{d}P/\mathrm{d}\xi \to -\lambda P$, where $\lambda = \sqrt{\epsilon^2/4+1} + \epsilon/2$. The parameter ϵ is positive for spin extraction and negative for spin injection. Using this asymptotic behaviour of $P(\xi)$ and equation (16) one can obtain a boundary condition for equation (18):

$$\lim_{P\to 0} \gamma/P = 1 - \lambda/\epsilon. \tag{19}$$

Solution of equation (18) with this boundary condition gives us a *universal* function $\gamma(P,\epsilon)$ which *uniquely* relates spin polarizations of the current and number densities at any spatial point of a semi-infinite quasi-neutral degenerate semiconductor or metal for any finite value of ϵ. Numerical solutions of equation (18) in the domain $0 \leqslant |P| \leqslant 1$ are shown in figure 2 for different values of ϵ. The parameter λ^{-1} is a dimensionless 'upstream' ($\epsilon > 0$, spin extraction) or 'downstream' ($\epsilon < 0$, spin injection) spin penetration length [48, 67]. As the current increases this length either tends to infinity, for spin injection, or to zero, for spin extraction.

This happens because the spin diffusion current is always directed away from the interface while the electric field and the drift current are either parallel (spin injection) or antiparallel (spin extraction) to it. As a result, the spin accumulation layer is either expanded away from the interface under spin injection or compressed towards the interface under spin extraction.

The physical situation corresponding to the spin extraction is shown in figure 4. In the forward-biased structure unpolarized electrons drift from the bulk of NS to the contact. Because of the spin selectivity of the contact the electrons with spin $\sigma = \uparrow$ (up electrons) are extracted from NS, i.e. $\delta n_\uparrow = (n_\uparrow - n_0/2) < 0$, and electrons with spin $\sigma = \downarrow$ (down electrons) are accumulated, i.e. $\delta n_\downarrow = (n_\downarrow - n_0/2) > 0$, near the contact. Here n_0, $n_\uparrow$ and $n_\downarrow$ are the equilibrium electron density in NS and densities of up and down electrons, respectively, at the boundary between the n$^+$-S layer and highly resistant NS region ($x = w$ in figure 4(a)). The quantity $|\delta n_\uparrow|$ increases with the electric field, E. In sufficiently strong fields, the drift efficiently compresses the spin polarized electrons to the boundary. As a result, the spin penetration length decreases with the current (cf white and dark curves in

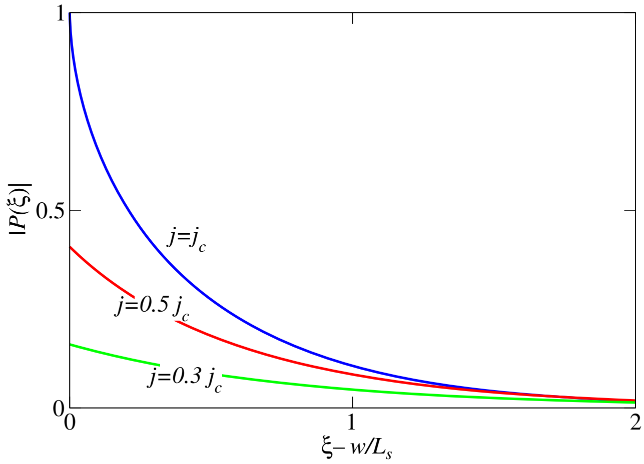

Figure 3. Spatial distribution of $P(\xi)$ (equation (17)).

figure 4(a)). Note that due to $\delta n_\downarrow = -\delta n_\uparrow$, the diffusion flow of up electrons is directed along the electron drift while the diffusion flow of down electrons is in the opposite direction; figure 4(a). The superlinear increase of the spin diffusion flows with the current can be compensated only by an increase of the spin density $n_\downarrow$ up to n_0 and a decrease of $n_\uparrow$ down to zero. In other words, the spin polarization of the electrons in NS near the FM–n$^+$-S contact $|P_w| = |\delta n_\uparrow - \delta n_\downarrow|/n_0 = 2|\delta n_\uparrow|/n_0$ can reach 100% when the current is sufficiently large.

As follows from equation (19) $\gamma/P \to 1$ as $\epsilon \to -\infty$ and $\gamma/P \to 0$ as $\epsilon \to \infty$. The solutions with $\gamma < 1$ and $|P| = 1$ do not exist for $\epsilon < 0$ but are possible for positive $\epsilon \geqslant \epsilon_c = 0.56$ (see figure 2). Therefore, the spin extraction in forward-biased FM–S junctions provides an opportunity to create a 100% spin polarized, non-equilibrium electron gas in a non-magnetic semiconductor near the FM–S interface. Whether or not such an opportunity can be realized depends on a particular physical system with specific boundary conditions. The goal of this article is to demonstrate that such systems are feasible and technologically sound.

Knowing $\gamma(P)$ we can easily find solutions of equation (17), $P(\xi) \equiv P_\xi$, by simple integration:

$$\xi - w/L_s = \int_{P_w}^{P_\xi} \frac{\tilde{D}(P)}{\epsilon(\gamma(P) - P)}\,\mathrm{d}P. \tag{20}$$

Some solutions of equation (17) are shown in figure 3. If function $P(\xi)$ reaches 1 at the interface it becomes singular, $|P| = 1 - C(\epsilon)\xi^{3/5}$, where $C(\epsilon) = 1.145 + 0.549\epsilon$ according to our numerical analysis. The spin polarization of the current density can be calculated as

$$\gamma = \frac{3}{5}\frac{C(\epsilon)^{5/3}}{\epsilon} - 1. \tag{21}$$

It follows from equation (21) that $|P|$ reaches 1 when $\gamma < 1$ provided that $j > 0.56 j_s$. One can see from figure 2 that the value of $|P| = 1$ can be achieved at rather small γ if the current is sufficiently large.

3. Boundary conditions

Let us consider the FM–n$^+$–n heterostructure (figure 1) based on GaAs. The thickness w of the n$^+$ layer with electron concentration $\sim 10^{19}$ cm^{-3} is about 10 nm and the electron concentration

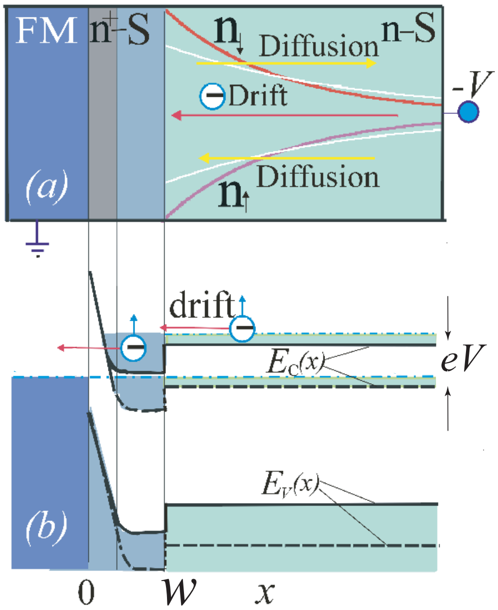

Figure 4. (a) Spatial distribution of spin-dependent non-equilibrium carrier densities in a non-magnetic semiconductor near a forward-biased FM–NS Schottky junction (spin extraction). (b) Corresponding band diagram in equilibrium (dashed lines) and under the bias (solid lines).

n_0 in the n-S region is in the range of 10^{17}–3×10^{17} cm^{-3}. We demonstrate that a 100% polarized spin accumulation layer is formed near the n$^+$–n interface $x = w$ when the forward current density reaches a critical value. The spin-dependent current across the FM–n$^+$ interface ($x = 0$) can be described using a generalized Landauer formula [71]:

$$j_\sigma(0) = \frac{e}{4\pi^2 h} \int \left[f(E-\zeta_\sigma) - f(E-F_\sigma) \right] T_\sigma(E, \vec{k}_\parallel, eV)\, \mathrm{d}\vec{k}_\parallel\, \mathrm{d}E. \tag{22}$$

Here ζ_σ and F_σ are the spin-dependent quasi-Fermi levels in n$^+$ and FM layers, respectively. We use the fact that the splitting of the quasi-Fermi levels in the superheavily doped n$^+$ layer is small compared to the Fermi energy E_F^+ in this region, i.e. $\Delta\zeta \ll E_F^+$ and $\Delta\zeta \propto P$. We consider low temperatures and neglect splitting of the quasi-Fermi levels in the FM metal. Also we use the local electroneutrality condition and assume that the Fermi level of the metal $F = 0$. Within this approximation $\zeta_\sigma = eV + \sigma\Delta\zeta/2$, where $\sigma = \pm 1$, and equation (22) reads

$$j_\sigma(0) = j_\sigma^{(0)}(V) + \tfrac{1}{2}\sigma\Sigma_\sigma(V)\Delta\zeta(0), \tag{23}$$

where

$$j_\sigma^{(0)}(V) = \frac{e}{4\pi^2 h} \int_{\max\{0, eV-E_F^+\}}^{eV} T_\sigma(E, \vec{k}_\parallel, eV)\, \mathrm{d}\vec{k}_\parallel\, \mathrm{d}E \tag{24}$$

$$\Sigma_\sigma(V) = \frac{e}{4\pi^2 h} \int_{\max\{0, eV-E_F^+\}}^{eV} T_\sigma(eV, \vec{k}_\parallel, eV)\, \mathrm{d}\vec{k}_\parallel. \tag{25}$$

Taking into account that $\Delta\zeta \propto P \ll 1$ in the n$^+$ layer we use the standard approximation in which $\Delta\zeta$ in this region satisfies a linear equation similar to equation (17) with $\tilde{D} = 1$ and $j = 0$ [64, 48, 67, 26]. Solving this equation we can express $\gamma(0)$ and $\Delta\zeta(0)$ through $\gamma(w)$ and $\Delta\zeta(w)$ by means of the following connection formulae:

$$\begin{pmatrix} \Delta\zeta(0)/2ejr_{\rm c} \\ \beta\gamma(0) \end{pmatrix} = \begin{pmatrix} \cosh\alpha & -\sinh\alpha \\ -\sinh\alpha & \cosh\alpha \end{pmatrix} \begin{pmatrix} \Delta\zeta(w)/2ejr_{\rm c} \\ \beta\gamma(w) \end{pmatrix}, \tag{26}$$

where $\alpha = w/L_N$, and L_N is the spin diffusion length in n^+ semiconductor.

Combining equations (23) and (26) we obtain the spin polarization γ on the n^+ side of interface $x = w$:

$$\gamma(w) = \frac{1}{\cosh\alpha + \beta\sinh\alpha}\left[\gamma_{\rm c} + \frac{j^{(0)}}{j}(\Gamma_{\rm c} - \gamma_{\rm c})\right] + \frac{1+\beta^{-1}\tanh\alpha}{1+\beta\tanh\alpha}\cdot\frac{\Delta\zeta(w)}{2ejr_{\rm c}}, \tag{27}$$

where $\Gamma_{\rm c} = \Delta j^{(0)}/j^{(0)}$, $\gamma_{\rm c} = \Delta\Sigma/\Sigma$, $r_{\rm c} = (\Sigma_\uparrow + \Sigma_\downarrow)/4\Sigma_\uparrow\Sigma_\downarrow$, $\beta = L_N\rho_N/r_{\rm c}$, and ρ_N is the resistivity of the n^+ semiconductor. The equation for the current density across the junction reads

$$j = j^{(0)}(V)\frac{1 - \Gamma_{\rm c}\gamma_{\rm c}}{1 - \gamma(0)\gamma_{\rm c}}. \tag{28}$$

We will assume that the resistivity of the n^+ region is tuned in such a way that $\beta \sim 1$. Also the transmission coefficient of an FM–n^+ junction can be represented as $T_\sigma = A_\sigma f(\vec{k}_\parallel, E)$ [62], where A_σ is determined by the density of states of electrons with spin σ in FM and weakly depends on E and $\vec{k}_\parallel$. This allows us to take A_σ out of the integrals in equations (24) and (25) and obtain compact expressions for the spin extraction coefficient $\gamma(w)$ and current density $j(V)$:

$$\gamma(w) = \frac{j^{(0)}(V)}{j}\left(1 + \frac{\Delta\zeta(w)}{2e}\frac{\mathrm{d}\ln j^{(0)}(V)}{\mathrm{d}V}\right) \tag{29}$$

$$j = j^{(0)}(V)\left(1 + \gamma_{\rm c}\frac{\Delta\zeta(w)}{2e}\frac{\mathrm{d}\ln j^{(0)}(V)}{\mathrm{d}V}\right) \tag{30}$$

where $\gamma_{\rm c} = \Delta\Sigma/\Sigma$ is the spin selectivity of the contact [52], $\Sigma = \Sigma_\uparrow + \Sigma_\downarrow$, $\Delta\Sigma = \Sigma_\uparrow - \Sigma_\downarrow$, and $j^{(0)} = j^{(0)}_\uparrow + j^{(0)}_\downarrow$. Using equation (12) and matching quasi-Fermi levels at the interface $x = w$ we obtain that in equations (29) and (30),

$$\Delta\zeta(w) = E_{\rm F}\left[(1+P_w)^{2/3} - (1-P_w)^{2/3}\right], \tag{31}$$

where P_w is the spin polarization of the electron density in the n-S region at $x = w$. Finally, we use the continuity of γ and match equation (29) with the solution of equation (18) in the n-S region. As a result we obtain spin polarization P_w, current density j, and spin extraction coefficient $\gamma(w)$ as functions of V. A typical dependence of P_w on j/j_s is shown in figure 5.

The critical current $J_{\rm c} = Sj_{\rm c}$, where S is the contact area, and voltage $V_{\rm c}$ needed to achieve $|P_w| = 1$ are determined by matching γ given by equations (29) and (21). The values of $J_{\rm c}$ and $V_{\rm c}$ required to completely spin polarize electrons of the density n_0 in n-GaAs near the n^+–n interface are shown in figure 6. We used a cubic approximation for $j^{(0)}(V)$ which is typical for tunnel contacts [72] since this approximation is well suited for Fe/GaAs and Fe/Si tunnel junctions studied experimentally in [57, 73]. The function $J^{(0)}(V) = Sj^{(0)}(V)$ with $S = 100\ \mu\mathrm{m}^2$ is shown in the inset to figure 6. This function corresponds to a triangular barrier of height 0.63 eV and the effective width of 1.38 nm. We also used $L_s = L_N = 1\ \mu$m, $\tau_s = 10^{-9}$ s, and $w = 10$–30 nm.

Once the dependences $\gamma(P)$ and $P(\xi) \equiv P_\xi$ are known one can recover a spatial dependence of any relevant physical quantity. In particular, the spatial dependence of the quasi-Fermi levels ζ_σ is of interest:

$$\zeta_\uparrow = \frac{1}{3}E_{\rm F}\int_{P_w}^{P_\xi}\frac{[\gamma(P) - P][1+\gamma(P)]}{(1+P)\tilde{D}(P)} + \zeta_\uparrow(w) \tag{32}$$

$$\zeta_\downarrow = \frac{1}{3}E_{\rm F}\int_{P_w}^{P_\xi}\frac{[\gamma(P) - P][1-\gamma(P)]}{(1-P)\tilde{D}(P)} + \zeta_\downarrow(w). \tag{33}$$

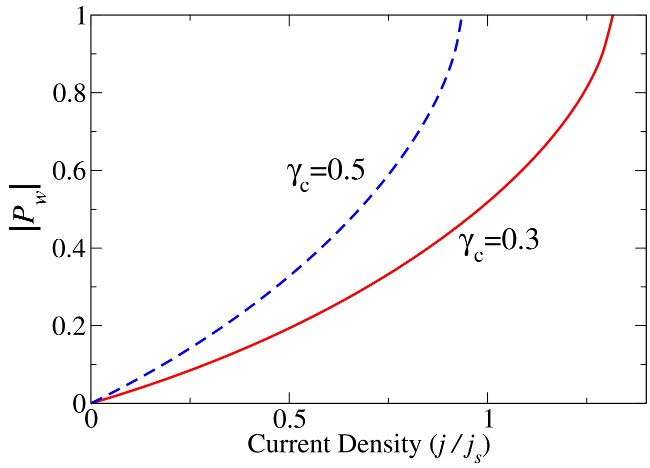

Figure 5. Current dependence of the spin polarization $|P_w|$ in n-S at the n^+/n interface.

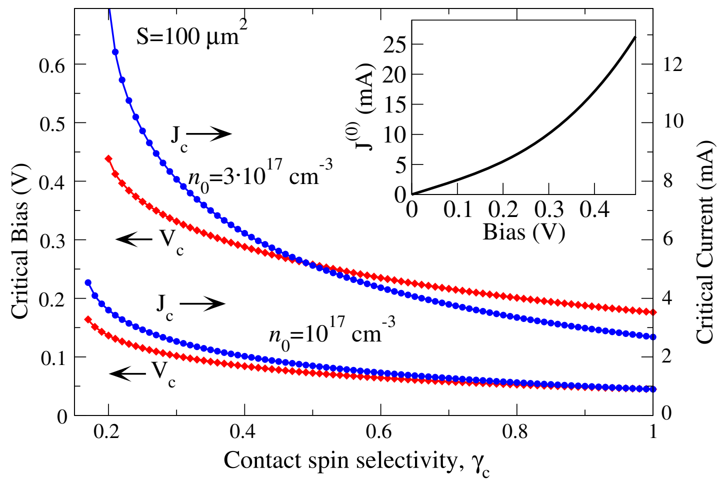

Figure 6. Critical currents and voltages.

The dependences of $\zeta_\uparrow(\xi)$ and $\zeta_\downarrow(\xi)$ are shown in figure 7 along with the electrostatic potential φ. The latter quantity displays a discontinuity which was first discussed in [74] (see also [52]). One can see that $\zeta_\downarrow(\xi)$ is a smooth function of ξ while the divergence of the first derivative of $\zeta_\uparrow(\xi)$ is notable.

We emphasize the crucial role of the n^+ layer in the proposed FM–n^+–n structure. The presence of the n^+ layer allows us to fabricate a very thin tunnel barrier which significantly reduces critical currents and voltages due to its low contact resistance. Moreover, the sharp concentration drop between the n^+ and n regions enables a dramatic change in the spin polarization of the n region while the n^+ region is only weakly perturbed. We notice that the transport across the n^+–n interface is diffusive. At the same time the concentration and the diffusion coefficient for the electrons with spin 'up' goes to zero. However, the spatial derivative of the concentration diverges and the diffusive current remains finite. It can be seen

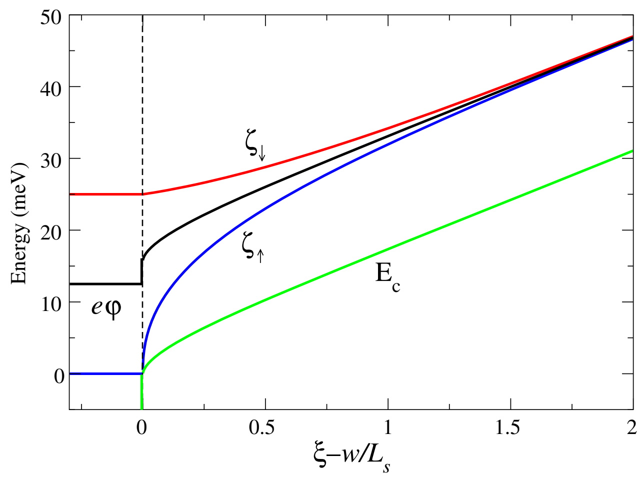

Figure 7. Calculated quasi-Fermi levels ζ_σ and electrostatic potential φ.

also from the divergence of the first derivative of the quasi-Fermi level $\zeta_\uparrow$ for the majority carriers near the interface (see figure 7) and equation (2). The effect of 100% spin accumulation cannot be realized in simple FM–n-S structures where a feedback occurs in the process of spin-dependent tunnelling [60–62].

Finally we would like to highlight some limitations of the theoretical approach presented here. First of all, our theory, which is based on the consideration of two non-equilibrium ensembles of the up and down electrons, becomes invalid when $n_\uparrow(w) \to 0$. Our approach is justified only when the time of electron–electron collisions within each of these systems is much less than τ_s. Second, at large currents $j > j_c$ the theory breaks down because the absolute value of the spin polarization, P_w, at the interface cannot exceed 1. The value of the spin polarization can be stabilized near $|P_w| \sim 1$ only if the total electron density $n = n_\uparrow + n_\downarrow$ exceeds its equilibrium value, n_0. Therefore, the condition of local electroneutrality will be violated and a space charge must accumulate near $x = w$ (see figure 1). This charge will change the electric field $E(x)$ and the total electron density in the vicinity of $x = w$. The drift–diffusion equations and Poisson's equation have to be solved self-consistently in this case. This regime must be investigated separately, which is beyond the scope of this paper. Our preliminary calculations show that, as expected, the characteristic scale of the non-uniform field region is determined by a relatively short screening length and the value of $|P_w|$ in the degenerate non-magnetic semiconductor remains very close to 1 near $x = w$ at $j \simeq j_c$.

4. Conclusions

In conclusion, we emphasize that we have demonstrated the possibility of achieving 100% spin polarization in NS via electrical spin extraction, using FM–n$^+$–n structures with moderate spin selectivity. The highly spin polarized electrons, according to the results of [75, 76], can be efficiently utilized to polarize nuclear spins in semiconductors. They can also be used to spin polarize electrons on impurity centres or in quantum dots located near the n$^+$–n interface. These effects are important for spin-based QIP [4, 28–30], including single-electron spin measurements [31] and quantum memory applications [29, 30]. The FM–n$^+$–n structures considered can be used as highly efficient spin polarizers or spin filters in a majority of the spin devices proposed to date [3, 4, 7, 24–27]. The effect of 100% spin polarization can be probed by means of the recently developed spin transport imaging technique [77].

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Appendix. Boundary conditions in the linear response case

It is instructive to see how the formalism of section 3 reproduces the results of the linear response theory of [52]. For the sake of simplicity let us consider a two-layer FM–NS structure with the interface between FM and NS at $x = 0$. Rashba's boundary conditions [52] can be expressed as

$$\Delta j(0) = \frac{\gamma_c r_c + \gamma_F r_F}{r_c + r_F} j + \frac{\Delta\zeta(0)}{2e(r_c + r_F)}. \tag{A.1}$$

Here $\Delta j(0) = j_\uparrow(0) - j_\downarrow(0)$ is the spin current density at the interface; $r_c = (\Sigma_\uparrow + \Sigma_\downarrow)/4\Sigma_\uparrow\Sigma_\downarrow$ and $r_F = L_F(\sigma_\uparrow + \sigma_\downarrow)/4\sigma_\uparrow\sigma_\downarrow$ are effective resistances of the interface and diffusion region in the ferromagnet respectively; $\gamma_c = (\Sigma_\uparrow - \Sigma_\downarrow)/(\Sigma_\uparrow + \Sigma_\downarrow)$ and $\gamma_F = (\sigma_\uparrow - \sigma_\downarrow)/(\sigma_\uparrow + \sigma_\downarrow)$ are corresponding spin polarizations; and $\Delta\zeta(0)$ is the splitting of the semiconductor quasi-Fermi levels at the interface given by equation (12) with $P = P_0$. Here P_0 is the spin polarization of the electron density in NS at the interface $x = 0$. Introducing $\gamma(0) = \Delta j(0)/j$ we can rewrite equation (A.1) as

$$\gamma(0) = \gamma_0 + \frac{3}{4}\frac{\epsilon_1}{\epsilon}\left[(1 + P_0)^{2/3} - (1 - P_0)^{2/3}\right]. \tag{A.2}$$

Here

$$\gamma_0 = \frac{\gamma_c r_c + \gamma_F r_F}{r_c + r_F} \tag{A.3}$$

and

$$\epsilon_1 = \frac{1}{3}\frac{m v_F^2}{e j_s (r_c + r_F)} = \frac{r_s}{r_c + r_F}, \tag{A.4}$$

where $r_s = L_s/\sigma_s$ is the effective resistance of the semiconductor spin diffusion region, and the conductivity $\sigma_s = e^2 n_0 \tau_{\mathrm{coll}}/m$.

In the limit of small currents (small ϵ), $P = P_0 \exp(-\xi)$, and equation (16) yields

$$\gamma(0) = -P_0/\epsilon. \tag{A.5}$$

On the other hand, we obtain from equation (A.2)

$$\gamma = \gamma_0 + \frac{\epsilon_1}{\epsilon} P_0. \tag{A.6}$$

This, in turn, yields

$$P_0 = -\frac{\epsilon}{\epsilon_1 + 1}\gamma_0 \tag{A.7}$$

and

$$\gamma(0) = \frac{\gamma_0}{\epsilon_1 + 1} = \frac{\gamma_c r_c + \gamma_F r_F}{r_c + r_F + r_s}. \tag{A.8}$$

This formula coincides with the linear response result of [52] for the spin injection coefficient.

If we consider a three-layer system of figure 1 the parameters in equation (A.1) will be renormalized but the mathematical structure of the matching conditions will remain the same. Using connection formulae similar to equation (26) we obtain

$$j_s(w) = \frac{1}{\cosh\alpha + \lambda\sinh\alpha}\frac{\gamma_c r_c + \gamma_F r_F}{r_F + r_c} j + \frac{\lambda^{-1}\sinh\alpha + \cosh\alpha}{\cosh\alpha + \lambda\sinh\alpha}\frac{\Delta\zeta(w)}{2(r_c + r_F)}. \tag{A.9}$$

Here $\lambda = r_N/(r_F + r_c)$, $r_N = L_N/\sigma_N$, $\alpha = w/L_N$. The quantities w, σ_N, and L_N are the thickness, conductivity and spin diffusion length of the n^+ region respectively. Assuming that $\alpha \ll 1$ we further obtain that $\gamma(w) \simeq \gamma(0)$, $\Delta\zeta(w) \simeq \Delta\zeta(0)$, and consequently $P_0 = P_w$, i.e. the spin polarizations of the current and electron densities are completely transferred from the FM–n^+ interface $x = 0$ to the n^+–n interface $x = w$. In this case we can simplify equation (A.9) as

$$\Delta j(w) = (1 - \lambda w/L_N)\gamma_c j + (1 + \lambda^{-1} w/L_N)\Delta\zeta(w)/2r_c \tag{A.10}$$

As previously, we consider the structures with $\lambda \sim 1$. In this case equations (A.10) and (A.1) are identical.

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