Complete spin polarization of degenerate electrons in semiconductors near ferromagnetic contacts

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Abstract

We show that spin polarization of electron density in nonmagnetic degenerate semiconductors can achieve 100%. This effect is realized in ferromagnet-semiconductor $FM-n^+-n$ junctions even at moderate spin selectivity of the $FM-n^+$ contact when the electrons are extracted from the heavily doped $n^+$-semiconductor into the ferromagnet. We derived a general equation relating spin polarization of the current to that of the electron density in nonmagnetic semiconductors. We found that the effect of the complete spin polarization is achieved near $n^+\text{--}n$ interface when an effective diffusion coefficient goes to zero in this region while the diffusion current remains finite.

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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 \cite{1,2}. The injection of spin-polarized electrons into nonmagnetic semiconductors (NS) is of particular interest because of the relatively large spin-coherence lifetime, $\tau_s$, and the promise for applications in both ultrafast low-power electronic devices \cite{1,2,3,4,5,6,7} and in quantum information processing (QIP) \cite{2,8,9,10,11}. Main characteristics of the spin injection are the spin polarizations of the electron density $P = (n^{\uparrow} - n^{\downarrow})/n = \Delta n/n$ and the current $\gamma = (j^{\uparrow} - j^{\downarrow})/j = \Delta j/j$. The value of $\gamma$ determines a magnetoresistance ratio and performance of spin-valve devices \cite{3,6,7,12,13}. The value of $P$ determines polarization of the recombination radiation measured in most of the experiments of optical detection of spin injection \cite{14,15,16}. Moreover, a high value of $P$ is crucial for QIP devices \cite{2,9,10}. It has been implied in most of the previous theoretical works on spin injection \cite{12,13,17,18,19,20,21,22,23,24} that $P$ cannot exceed $\gamma$. This assumption complies 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 \cite{1,2}.

It follows from a formal consideration by Yu and Flatte \cite{20,21} that $P$ can, in principle, exceed $\gamma$ in nondegenerate semiconductors when electron spins are extracted from NS into FM (reverse bias). However, more detailed studies by Osipov and Bratkovsky \cite{6,7}, taking into account tunneling through a Schottky barrier in simple FM-NS junctions, revealed that $P < \gamma$ due to a feedback formed during the tunneling process. The condition $P < \gamma$ holds for both nondegenerate and degenerate semiconductors and for both reverse- and forward-biased simple FM-NS junctions \cite{23,24,25}.

Unlike previous works where simple FM-NS junctions were studied, in this Letter we consider a band-engineered FM-$n^+\!-\!n$ structure containing a thin super-heavily doped $n^+$-layer and a degenerate semiconductor $n$-region (Fig. 1). The effect in question is based on spin extraction and nonlinear dependence of the nonequilibrium 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 $n^+\!-\!n$ interface. The spin extraction from NS was predicted by I. Zutic et al. \cite{26} for forward-biased $p\!-\!n$ junctions containing a magnetic semiconductor, was studied in detail for FM-NS junctions \cite{3,7}, and was experimentally found in forward-biased MnAs/GaAs Schottky
junction [27]. However, both the predicted and observed values of the spin polarization $P$ were rather small.

![Diagram of proposed FM-n$^+$ – n heterostructure](image)

**FIG. 1:** (Color online.) Schematic view of the proposed FM-n$^+$ – n heterostructure. Inset: calculated $\zeta_\sigma$ and electrostatic potential $\varphi$ at $j = j_c$.

Let us consider a nonmagnetic semiconductor in which non-equilibrium spin-polarized electrons are described by the quasi-Fermi distribution and the current density $j_\sigma$ can be expressed as:

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

(1)

where $E$ is the electric field, $\mu = e\tau_p/m$ is the mobility, $\tau_p$ is the momentum relaxation time, $m$ is the effective mass and $D_\sigma$ is the diffusion coefficient of electrons with spin $\sigma$. Here we used the generalized Einstein’s relation [28] $\mu = eD_\sigma \partial\ln(n_\sigma)/\partial\zeta_\sigma$. Since $\mu$ is spin independent this relation shows that $D_\sigma$ does not depend on spin in nondegenerate semiconductors ($n \propto \exp(-\zeta_\sigma/kT)$) while the spin dependence of $D_\sigma$ is crucial for degenerate semiconductors.
Using Eq. (1) and \( j = \text{const} \) in steady-state we find:

\[
\gamma = P + (1 - P^2) \frac{\mu n \partial \Delta \zeta}{2j} \frac{\partial}{\partial x}
\]

(2)

where \( \Delta \zeta = \zeta^\uparrow - \zeta^\downarrow \). It follows that \( \gamma = P \) only in the absence of diffusion. Therefore the term \( P \) in this equation can be interpreted as a spin-drift term while the other one as a spin-diffusion term.

We consider the FM-\( n^+ \)-\( n \) structure shown in Fig. 1. We note that the sign of \( \gamma > 0 \) is independent of the direction of the current while the sign of \( P \) does depend on it. Namely, \( P > 0 \) for reverse-biased junctions (total current \( j = (j^\uparrow + j^\downarrow) < 0 \) when the spin injection occurs and \( P < 0 \) for forward-biased junctions ( \( j > 0 \) when the spin extraction takes place. Due to very high electron density we use the electro-neutrality condition, \( n = n_0 \), where \( n_0 \) is the equilibrium electron density. In this case Eq. (2) reduces to:

\[
\gamma = P + \frac{en_0 D(P) dP}{j} \frac{\partial}{\partial x},
\]

(3)

where

\[
D(P) = \frac{\mu}{2e} (1 - P^2) \frac{\partial \Delta \zeta(n_0, P)}{\partial P}
\]

(4)
is a bi-spin diffusion coefficient. For degenerate semiconductors at low temperatures

\[
\Delta \zeta = E_F \left[(1 + P)^{2/3} - (1 - P)^{2/3}\right],
\]

(5)

where \( E_F = mv_F^2/2 \) is the equilibrium Fermi energy and \( v_F = (h/m)(3\pi^2n_0)^{1/3} \). From Eqs. (4)-(5) we obtain

\[
D(P) = (v_F^2 \tau_p/3) \tilde{D}(P),
\]

(6)

where

\[
\tilde{D}(P) = \frac{1}{2} (1 - P^2)^{2/3} \left[(1 + P)^{1/3} + (1 - P)^{1/3}\right]
\]

(7)
The steady-state continuity equation for spin-dependent currents in NS reads:

\[
\frac{dj_\sigma}{dx} = \frac{e}{2\tau_\sigma} (n_\sigma - n_{-\sigma}).
\]

(8)

Introducing the spin diffusion length \( L_s^2 = (v_F^2 \tau_p \tau_s)/3 \) and dimensionless length \( \xi = x/L_s \), from Eqs. (8) and (3) we find:

\[
\frac{\dot{j}}{j} \frac{d\gamma}{d\xi} = P, \text{ where } \gamma = P + \frac{j \tilde{D}(P) dP}{j} \frac{\partial}{\partial \xi}
\]

(9)
and $j_s = e n_0 L_s / \tau_s$. We remember that $j$ is positive for spin extraction and negative for spin injection. System of Eqs. (9) leads to a non-linear drift-diffusion equation in dimensionless variables:

$$\frac{d}{d\xi} \left( \tilde{D}(P) \frac{dP}{d\xi} \right) + \frac{j}{j_s} \frac{dP}{d\xi} - P = 0,$$

Eliminating $dP/d\xi$ from Eq. (9) we can reduce the second-order non-linear equation (10) to the first-order equation relating $\gamma$ to $P$:

$$\frac{j^2}{j_s^2} \frac{d\gamma}{dP} = \tilde{D}(P) \frac{P}{\gamma - P}.$$  

We notice that $\tilde{D}(P) = \text{const}$ in nondegenerate semiconductors and solution of Eq. (11) reduces to the known result [6, 20, 21]. A boundary condition for Eq. (11) can be obtained from the asymptotics $P \to 0$ and $dP/d\xi \to -P/l_j$ at $\xi \to \infty$, where $l_j^{-1} = \sqrt{j^2/4j_s^2 + 1 + j/2j_s}$. Using these asymptotics and Eqs. (9) we find the boundary condition for Eq. (11):

$$\lim_{P \to 0} \frac{\gamma}{P} = 1 - j_s/j_l.$$

Solution of Eq. (11) with this boundary condition is a universal function $\gamma(P, j)$ determining local relation between $\gamma$ and $P$. Numerical solutions of Eq. (11) in the domain $0 \leq |P| \leq 1$ are shown in Fig. 2 for different values of $j$.

The parameter $l_j$ is a dimensionless spin penetration length [6, 17, 20, 21]. This length at large currents tends to infinity for spin injection ($j < 0$) or to zero for spin extraction ($j > 0$). It means that the spin accumulation layer is expanded away from the interface under spin injection and compressed towards the interface under spin extraction. As it follows from Eq. (12) $\gamma/P \to 1$ at $j \to -\infty$ and $\gamma/P \to 0$ at $j \to \infty$. A solution with $|P| = 1$ does not exist for $j < 0$ and $\gamma < 1$ but is possible for positive $j \geq 0.56j_s$ (see Fig. 2). Therefore, the spin extraction in forward-biased FM-S junctions provides a possibility to create a 100% spin-polarized, non-equilibrium electron gas in a non-magnetic semiconductor near the FM-S interface. In this Letter we demonstrate that this possibility is feasible and technologically sound. Solutions of Eq. (11) for spatial distributions of $P(\xi)$ in n-S-region (Fig. 1) are shown in the inset to Fig. 2. The function $|P(\xi)|$ reaches 1 at the interface and becomes singular when $j = j_c > 0.56j_s$. The value of $j_c$ depends on boundary conditions and will be calculated below. Our numerical analysis shows that at this point $|P| = 1 - C(j)(\xi - w/L_s)^{3/5}$, where $C(j) = 1.145 + 0.549j/j_s$. The current spin polarization at $\xi = w/L_s$ equals to:

$$\gamma = (3/5)(j_s/j)C(j)^{5/3} - 1$$
FIG. 2: (Color online.) Solutions of Eq. (11) for different \( j \). Inset: spatial distribution of \( P(\xi) \)

It follows from Eq. (13) that \( |P| \) reaches 1 when \( \gamma < 1 \) provided that \( j > 0.56j_s \). One can see from Fig. 2 that the value of \( |P| = 1 \) can be achieved at rather small \( \gamma \) if the current is sufficiently large.

Let us consider the FM-\( n^+ - n \) heterostructure (Fig. 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 \( n_0 \) in \( n - S \) region is in the range of \( 10^{17} - 3 \cdot 10^{17} \) cm\(^{-3}\). We demonstrate that a 100%-polarized spin accumulation layer is formed near \( n^+ - n \) interface \( x = w \) when the
forward current density reaches a critical value. The spin-dependent current across FM-n\(^+\) interface \((x = 0)\) can be described by a generalized Landauer formula \([29]\):

\[
j_\sigma(0) = \frac{e}{4\pi^2 h} \int [f(E - \zeta_\sigma) - f(E - F_\sigma)] T_\sigma(E, \vec{k}_\|, eV) d\vec{k}_\| dE
\]

(14)

Here \(\zeta_\sigma\) and \(F_\sigma\) 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 super-heavily doped \(n^+\) layer is small compare to the Fermi energy \(E_F^\pm\) in this region, i.e. \(\Delta \zeta \ll E_F^\pm\) 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 electro-neutrality 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 Eq. (14) reads:

\[
j_\sigma(0) = j_\sigma^{(0)}(V) + \frac{1}{2} \sigma \Sigma_\sigma(V) \Delta \zeta(0), \text{ where}
\]

(15)

\[
j_\sigma^{(0)}(V) = \frac{e}{4\pi^2 h} \int_{\max\{0, eV - E_F^+\}}^{eV} T_\sigma(E, \vec{k}_\|, eV) d\vec{k}_\| dE
\]

(16)

\[
\Sigma_\sigma(V) = \frac{e}{4\pi^2 h} \int_{\max\{0, eV - E_F^+\}}^{eV} T_\sigma(eV, \vec{k}_\|, eV) d\vec{k}_\|
\]

(17)

Taking into account that \(\Delta \zeta \propto P << 1\) in the \(n^+\)-layer we use the standard approximation in which \(\Delta \zeta\) in this region satisfies a linear equation similar to Eq. \([10]\) with \(\tilde{D} = 1\) and \(j = 0\) \([6, 17, 21, 21]\). By solving this equation we can express \(\gamma(0)\) and \(\Delta \zeta(0)\) through \(\gamma(w)\) and \(\Delta \zeta(w)\). The transmission coefficient of an FM-\(n^+\) junction can be represented as \(T_\sigma = A_\sigma f(\vec{k}_\|, E)\) \([25]\), where \(A_\sigma\) is determined by the density of states of electrons with spin \(\sigma\) in FM and weakly depends on \(E\) and \(\vec{k}_\|\). It allows us to take \(A_\sigma\) out of the integrals in Eqs. \([16]\) and \([17]\) and obtain compact expressions for spin extraction coefficient \(\gamma(w)\) and current density \(j(V)\):

\[
\gamma(w) = \frac{j^{(0)}(V)}{j} \left(1 + \frac{\Delta \zeta(w) d\ln j^{(0)}(V)}{2e dV} \right)
\]

(18)

\[
j = j^{(0)}(V) \left(1 + \gamma_c \frac{\Delta \zeta(w) d\ln j^{(0)}(V)}{2e dV} \right)
\]

(19)

where \(\gamma_c = \Delta \Sigma / \Sigma\) is the spin selectivity of the contact \([12]\), \(\Sigma = \Sigma_\uparrow + \Sigma_\downarrow\), \(\Delta \Sigma = \Sigma_\uparrow - \Sigma_\downarrow\), and \(j^{(0)} = j^{(0)}_\uparrow + j^{(0)}_\downarrow\). Using Eq. \([5]\) and matching quasi-Fermi levels at the interface \(x = w\) we obtain that in Eqs. \([18]\) and \([19]\), \(\Delta \zeta(w) = E_F \left[(1 + P_w)^{2/3} - (1 - P_w)^{2/3}\right]\), where \(P_w\) is the spin polarization of the electron density in \(n\)-\(S\) region at \(x = w\).
continuity of \( \gamma \) and match Eq. (18) with the solution of Eq. (11) in \( n - S \) 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 Fig. 3.

The critical current \( J_c = S j_c \), where \( S \) is the contact area, and voltage \( V_c \) needed to achieve \( |P_w| = 1 \) are determined by matching \( \gamma \) given by Eqs. (18) and (13). The values of \( J_c \) and \( V_c \) required to completely spin polarize electrons of the density \( n_0 \) in \( n \)-GaAs near \( n^+ - n \)-interface are shown in Fig. 4. We used a cubic approximation for \( j^{(0)}(V) \) which is typical for tunnel contacts [30] since this approximation is well suited for Fe/GaAs and Fe/Si tunnel junctions studied experimentally in [15, 31]. The function \( J^{(0)}(V) = S j^{(0)}(V) \) with \( S = 100 \mu m^2 \) is shown in the inset to Fig. 4. This function corresponds to a triangular barrier of the height of 0.63 eV and the effective width of 1.38 nm. We also used \( L_s = L_s^+ = 1 \mu m \), \( \tau_s = 10^{-9} \) s, and \( w = 10-30 \) nm.

We emphasize the crucial role of the \( n^+ \) layer in the proposed FM-\( n^+ - n \) structure. The presence of \( n^+ \)-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 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. This effect cannot be realized in simple FM-$n-S$ structures where a feedback occurs in the process of spin-dependent tunneling [23, 24, 25].

![Graph showing critical bias and currents](image)

**FIG. 4:** (Color online.) Critical currents and voltages

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 Refs. [32, 33], can be efficiently utilized to polarize nuclear spins in semiconductors. They can also be used to spin polarize electrons on impurity centers or in quantum dots located near the $n^+$-$n$ interface. These effects are important for spin-based QIP [2, 8, 9, 10], including single electron spin measurements [11] and quantum memory applications [9, 10]. The considered
FM-$n^+\text{-}n$ structures can be used as highly efficient spin polarizers or spin filters in a majority of the spin devices proposed to date \[1, 2, 3, 4, 5, 6, 7\]. The effect of 100% spin polarization can be probed by means of the recently developed spin transport imaging technique \[34\].

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