Optimized spin-injection efficiency and spin MOSFET operation based on low-barrier ferromagnet/insulator/n-Si tunnel contact

Yang Yang1, Zhenhua Wu2, Wen Yang3, Jun Li1,*, Songyan Chen1, and Cheng Li1

1Department of Physics, Semiconductor Photonics Research Center, Xiamen University, Xiamen 361005, China
2Key Laboratory of Microelectronic Devices and Integrated Technology, Institute of Microelectronics, Chinese Academy of Sciences, 100029 Beijing, China
3Beijing Computational Science Research Center, Beijing 100089, China

*E-mail: ljun@xmu.edu.cn

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We theoretically investigate the spin injection in different ferromagnet/insulator/n-Si tunnel contacts by using the lattice non-equilibrium Green’s function method. We find that the tunnel contacts with low-barrier materials such as TiO2 and Ta2O5 have far lower resistances than the conventional-barrier materials, resulting in a wider and attainable optimum parameters window for improving the spin-injection efficiency and magnetoresistance ratio of a vertical-spin metal–oxide–semiconductor field-effect transistor. Additionally, we find that the spin-asymmetry coefficient of the TiO2 tunnel contact has a negative value, while that of the Ta2O5 contact can be tuned between positive and negative values by changing the parameters. © 2017 The Japan Society of Applied Physics

The spin degrees of freedom have drawn attention from researchers because they shed lights on next-generation devices with novel charge-spin integrated functionalities.1,2 Realizing spin-based electronics (spintronics) on silicon, i.e., the most widely used material in the semiconductor industry, has special significance because the established mature Si technology can greatly facilitate the production and widespread application of spintronic devices. Fortunately, silicon is considered as an ideal host for spintronics, as it exhibits a long spin lifetime and diffusion length.3,4 There has been remarkable progress in Si-based spintronics in the past decade. Room-temperature electrical spin injection in silicon through ferromagnet/insulator/Si (FM/I/Si) tunnel contacts with Al2O3, SiO2, and crystalline MgO as barriers were reported.3–5 Spin-polarized signals were detected by local three-terminal (3T)3,4 and non-local four-terminal (NL-4T)5 Hanle measurements, and the spin transport in Si channel were demonstrated in a spin metal–oxide–semiconductor field-effect transistor (MOSFET).6,7 Nevertheless, there remain challenges in obtaining clear and reliable signals, as well as understanding the spin-transport process in the FM/I/Si tunnel contacts. The local 3T Hanle signals have been under intensive debate since they were recently found to be dominated by the defect-states-assisted hopping8,9 rather than by the spin accumulation in silicon. The spin signals of NL-4T spin MOSFETs are very weak,6,7 implying that further optimizations of the FM/I/Si contacts are required for their practical use in spintronic devices.

As reported by Fert et al., a noticeable spin signal caused by the spin injection from a ferromagnet into a semiconductor can be observed only if the contact resistance is engineered into an optimum window,5,10 the contact resistance cannot be too low to overcome the conductivity mismatch10 or too high to keep the electron dwell time shorter than the spin lifetime.11 Min et al. revealed that the resistances of conventional tunnel contacts are orders of magnitude higher than the optimum value, owing to the formation of the Schottky barrier.12 Therefore, maintaining a low contact resistance is very important for enhancing the spin signals. As a low-resistance material, graphene has been demonstrated as a good tunnel layer for efficient spin injection into silicon.13 It is reasonable to expect that other low-barrier materials, such as TiO2 and Ta2O5, can also be used as low-resistance tunnel barriers for improving the spin-injection efficiency. These low-barrier materials have the advantage of compatibility with the established Si technology. Additionally, their thickness can be adjusted, which offers the ability to tune the contact resistance and suppress the formation of paramagnetic silicide.2,3 However, the spin-transport process in the low-barrier tunnel contact is much complicated, because both the Schottky barrier and the thermionic emission can play important roles. Therefore, a unified model that considers these effects is necessary for studying the spin transport of low-barrier FM/I/Si tunnel contacts.

In this paper, we present a theoretical investigation of the spin injection in different FM/I/n-Si tunnel contacts via the non-equilibrium Green’s function (NEGF) method.14,15 The transmission coefficient of band profiles with various tunnel and Schottky barriers are calculated using the lattice Green’s function. The thermionic emission process is considered according to the temperature-dependent Fermi energy of n-Si and the Fermi–Dirac distributions. Via this method, the spin polarization (SP) of the injected current, its parameter dependence, and the magnetoresistance (MR) ratio of a vertical-spin MOSFET16 are examined.

The model of the FM/I/n-Si tunnel contact is illustrated in Fig. 1(a). The contact region [Z0, Z1] is assumed to be located between two semi-infinite leads, z ∈ [Z0, Z1], [Z1, Z2], and (Z2, Z3), correspond to the ferromagnet, insulator barrier, and n-Si, respectively. Similar to the two-current model,17 the electrons with majority (↑) and minority (↓) spin can be regarded as flowing in independent channels. In the contact region, the Hamiltonian operator for each spin channel is

\[
\hat{H}_c^\sigma = -\frac{\hbar^2}{2m^\sigma} \left[ \frac{1}{m_1^\sigma(z)} \frac{\partial}{\partial z} \right] + \frac{\hbar^2 k^\sigma_1}{2m_1^\sigma(z)} + U^\sigma(z),
\]

where \( \sigma \in \{ \uparrow, \downarrow \} \) is the index of the spin, \( \hbar \) is the reduced Planck constant, \( k_1 \) is the transverse wave vector, and \( m_1^\sigma(z) \) is the material-dependent transverse (longitudinal) electron effective mass. Here, we assume the electron effective mass \( m_{1,e}^\sigma \) of the ferromagnet (insulator) is isotropic, while the electron effective mass of n-Si is anisotropic, and \( m_{1,n}^\sigma(z) \) is the transverse (longitudinal) electron effective mass of n-Si.
Fig. 1. (a) Schematic of the energy band profile of a FM/I/n-Si tunnel contact under a reverse bias \(V_A < 0\) for the spin injection. The inset of (a) depicts the vertical-spin MOSFET with a symmetric FM/I/n-Si/I/FM multilayer structure. (b, c) Typical results of the averaged transmission coefficient \(T(V_A = 0.2 \text{ V} \text{ and } k = 0)\) and the total current density \(J\) \((d_1 = 1 \text{ nm}, J_{D0} = 3 \times 10^{13} \text{ cm}^{-2} \text{ s}^{-1}, \text{ and } T_0 = 300 \text{ K})\), respectively.

**U^\sigma(z)** denotes the potential energy–profile function for the \(\sigma\) spin channel and consists of two parts:

\[
U^\sigma(z) = U^\sigma_{CBO}(z) + U^\sigma_{S}(z).
\]

\(U^\sigma_{CBO}(z)\) describes the profile of the conduction-band offset for \(\sigma\) spin and depends on the conduction-band bottom of the ferromagnet \(E^C_{F}\) and the electron affinity \(\chi_S\) of the insulator barrier (n-Si). Because of the exchange interaction, \(E^C_{F}\) is split by the exchange splitting energy \(\Delta\). \(U^\sigma_S(z)\) describes the spin-independent Schottky barrier energy profile, which is induced by the charge accumulation near the FM/I and I/n-Si interfaces. By using the standard deplleton-layer approximation, \(U^\sigma_S(z)\) is determined by the work function of the ferromagnet \(\phi_m\), the electron affinity \(\chi_S\) of n-Si, the doping density \(N_D\), the thickness of the insulator barrier \(d_i\), the permittivity of the insulator (n-Si) \(\varepsilon_i\) \((\varepsilon_S)\), and the Fermi energy \(E_{FS}\) of n-Si. For n-Si from the non–degenerate regime to the degenerate regime, \(E_{FS}\) depends on the doping density \(N_D\) and the temperature \(T_0\) and can be determined by numerically solving the charge neutrality condition. At thermal equilibrium, the Fermi energy \(E_{FS}\) of the ferromagnet is equal to \(E_{FS}\). If the contact is under an applied bias of \(V_A\), \(E_{FS} = E_{FS} + qV_A\), where \(q\) is the elementary charge of an electron. Note that for a reverse (forward) bias, i.e., \(V_A < 0\) \((V_A > 0)\), the tunnel contact is in the spin-injection (extraction) mode.

By discretizing the contact region into a uniformly spaced one-dimensional grid with spacing of \(a\), the Hamiltonian operator \(\hat{H}^a_C\) can be transformed into a \(N \times N\) tridimensional matrix \(H^a_C\) by the method of finite differences, where \(N\) is the total number of grid points. The retarded Green’s function in the lattice representation can be expressed as follows:

\[
G^\sigma_C = (E + i\eta)I - H^\sigma_C - \Sigma^\sigma_L - \Sigma^\sigma_R)^{-1},
\]

where \(E\) is the electron transmission energy, \(I\) is the identity matrix, and \(\eta\) is an infinitesimally small positive number. The coupling of the contact to the left (right) semi-infinite lead is considered by a \(N \times N\) matrix of the self-energy:

\[
\Sigma^\sigma_{L(R)} = \begin{pmatrix} \Sigma_{ij} & 0 \\ 0 & 0 \end{pmatrix}
\]

for \(i = j = 1(N)\),

\[
\text{otherwise}
\]

where \(\Sigma^\sigma_{L(R)}(2m_i^2(z_{2N}+1)) = \{E - E_i(z_{2N}+1) - U^\sigma(z_{2N})\}/\hbar\) is the longitudinal wave vector of an electron with \(\sigma\) spin in the left (right) lead, \(E = E_i(z_{2N}+1)\) is the transverse kinetic energy of an electron, and \(t_i = h^2/2m_i^2(z_{2N+1})\) is the coupling strength between the nearest grid points. In these expressions, \(z_n\) denotes the coordinate of the \(n\)-th grid point. \(z_0\) and \(z_{N+1}\) are the coordinates of the first point in the left and right leads, respectively. The transmission coefficient of the \(\sigma\) spin channel can be given by the NEGF formalism as

\[
T^\sigma(k_i, E) = Tr[\Gamma^\sigma_L G^\sigma_C \Gamma^\sigma_R G^\sigma_S],
\]

where \(\Gamma^\sigma_{L(R)} = \{[\Sigma^\sigma_{L(R)} - \Sigma^\sigma_{L(R)}] \times \exp(-i\pi/2)\} \) is the broadening matrix. The current density of the \(\sigma\) spin channel is then calculated using the Landauer formula:

\[
J^\sigma = -\frac{2}{\pi\hbar} \int_0^{E_F} T^\sigma(k_i, E)[f_L(E) - f_R(E)]k_i dk_i dE,
\]

where \(f_{L,R}(E) = 1/[e^{(E-E_F)/k_BT_0}] + 1\) is the Fermi–Dirac distribution function in the left (right) lead, and \(k_B\) is the Boltzmann constant.

For a contact with a potential profile consisting of an insulator barrier band offset and a space–varying Schottky barrier, \(T^\sigma\) and \(J^\sigma\) can be calculated using Eqs. (5) and (6), respectively. For the low tunnel barriers, a portion of free electrons can be thermally exited [determined by \(f_{L,R}(E)\)], even to obtain higher energies over the barrier, so that \(T^\sigma\) is close to 1. The transport of these electrons is not by tunneling but by the thermionic emission and is automatically considered in this model. The typical results of the averaged transmission coefficient of the two spin channels, i.e., \(\bar{T} \equiv (T^\sigma + T^{-\sigma})/2\), and the total electric current density, i.e., \(J \equiv J^\sigma + J^{-\sigma}\), are shown in Figs. 1(b) and 1(c), respectively. We observe the exponentially varying feature of \(\bar{T}\) and the current-rectifying effect of the Schottky contact is well-reproduced by our calculations. For the contact in the spin-extraction mode, although the calculated \(SP\) is 25–60% smaller, the spin-injection efficiency is generally higher than that in the spin-injection mode. When \(V_A > 0\), the depletion region is suppressed, and the contact resistance can be reduced by orders of magnitude to alleviate the spin depolarization. In the following part, we focus on the tunnel contacts in the spin-extraction mode, e.g., for \(V_A = 40.2 \text{ V}\).

In the calculations, we assume that the contact is grown along the [001]-orientation of silicon; thus, \(m_{Si} = 0.20\) \((0.92)\) \(m_e\) \((300 \text{ K})\), \(\varepsilon_i = 11.5 \varepsilon_0\) and \(\chi_S = 4.2 \text{ eV}\), where \(m_e\) and \(\varepsilon_0\) are the free electron mass and the permittivity of vacuum, respectively. The ferromagnet material is chosen to be Fe, whose parameters are \(\phi_m = 4.5 \text{ eV}\), \(m^*_{Fe} = 2.3 m_e\), and \(\Delta = 1.5 \text{ eV}\). These parameters can recover the Fermi wave vector \(k^F_{\uparrow} = 1.05 (0.44) \text{ Å}^{-1}\) for the \(\uparrow (\downarrow)\) spin of Fe.

The parameters for different insulator barriers are listed in Table I. The effective–resistance–area (RA) product \(r^2_B\) of the tunnel contact and the spin-asymmetry coefficient (of the contact resistance) \(\gamma\) is given as follows:

\[r^2_B = \frac{4}{\pi} \frac{k_B T_0}{J^\sigma} \ln \frac{J^\sigma}{J^{-\sigma}}.
\]

\[\gamma = \frac{J^{-\sigma}}{J^\sigma}.
\]
accumulation should be described by the spin drift-diffusion transport, can hardly be prevented from forming with respect to the doping density, such a thin layer (except for TiO$_2$ with a 0-eV barrier height) will prevent the injected current from being tunable to balance the required resistances and the contact quality.

For SiO$_2$, Al$_2$O$_3$, and AlN contacts with $d_i > 0.5$ nm, the SP of the injected current is almost independent of $N_D$ and $d_i$ [see Figs. 2(b) and 2(d)]. The reason is that the $r_\sigma^b$ of these contacts is far larger than the spin resistance $r_N (\equiv \rho_N l_D^N)$ of n-Si, causing the SP to be saturated at SP = $\gamma \approx 0.17$–0.2. For low-barrier tunnel contacts, the behavior of the SP vs $N_D$ and $d_i$ differs significantly. We observe that the SP of the TiO$_2$ contact has a negative value; i.e., the polarization direction of the injected spins in silicon is opposite to that in the ferromagnet. This is because the minority spin in the ferromagnet has a smaller $\Delta E_F$ than the majority spin, which better matches the small evanescent wave vector ($\alpha \sqrt{\Delta E_F - E}$) inside the TiO$_2$ barrier, leading to a larger $T^1$ than $T^{-1}$. Thus, for the TiO$_2$ contact, $J^1$ is larger than $J^{-1}$, and a negative $\gamma$ (or SP) is produced. In contrast, for conventional barriers such as SiO$_2$, Al$_2$O$_3$, and AlN, the majority spin matches the evanescent wave vector better, which makes $T^1$ larger than $T^{-1}$ and $\gamma$ (or SP) be positive.

To demonstrate this, Fig. 3(a) plots the difference of the transmission coefficient between the two spin channels, i.e., $\Delta T \equiv T^1 - T^{-1}$, with respect to the electron transmission energy $E$. The black dashed line in this figure represents the difference of the Fermi–Dirac distribution functions, i.e., $\Delta f_\sigma(E) \equiv f_\sigma(E) - f_{\bar{\sigma}}(E)$, which determines the contribution of an electron with energy $E$ to the current. From $\Delta f_\sigma(E)$, we observe that the effective energy range is $0 < E < 0.16$ eV. For $E$ outside of this range, the contribution of $\Delta f_\sigma(E)$ falls below $10^{-4}$. Because the $\Delta T$ of TiO$_2$ is negative in this range, $\gamma$ is negative. For other barriers (with $d_i = 1$ nm), the $\Delta T$ values in this range are positive; thus, their $\gamma$ values are also positive. Interestingly, we find that the $\gamma$ (or SP) for Ta$_2$O$_5$ can be tuned from positive to negative by decreasing $d_i$, as shown in Fig. 2(d). The reason for the sign change of $\gamma$ is illustrated in Fig. 3(b): the positive (negative) region of $\Delta T$ shrinks (expands) with decreasing $d_i$. By changing the temperature, the broadening of $\Delta f_\sigma(E)$ can be varied, resulting in the $\gamma$ for Ta$_2$O$_5$ be more sensitively dependent on the temperature compared with other barriers [see Fig. 3(c)]. For a 0.5-nm-thick Ta$_2$O$_5$ contact, $\gamma$ can be tuned from positive to negative by increasing the temperature. For TiO$_2$, $\gamma$ exhibits a non-monotonic dependence on the temperature. This is ascribed to

![Fig. 2](image-url)  
(a, b) Dependence of $r_\sigma^b$ and SP with respect to the doping density $N_D$ of n-Si for FM/I/n-Si contacts with different insulator barriers ($d_i = 1$ nm). (c, d) The same as (a) and (b), but as a function of the thickness of the barrier $d_i (N_D = 5 \times 10^{16}$ cm$^{-3}$). $V_\text{As} = 0.2$ V (spin extraction mode) and $T_0 = 300$ K are assumed in this figure.

![Fig. 3](image-url)  
(a) $\Delta T$ as a function of the electron transmission energy $E$ for different tunnel contacts ($V_\text{As} = 0.2$ V, $d_i = 1$ nm, and $T_0 = 300$ K). (b) Same as (a), but for a Ta$_2$O$_5$ contact with a different $d_i$. The black dash-dot, dashed, and dash-dot-dot lines represent $\Delta f_\sigma(E)$ at 150, 300, and 450 K, respectively. (c) $\gamma$ with respect to the temperature $T_0$ for different tunnel contacts. (d) $P_{\text{eff}}$ and $\gamma$ with respect to the tunnel barrier height $\Delta E_{\text{si}} - E$ (except for TiO$_2$ with a 0-eV barrier height) is illustrated in Fig. 3(c).
MOSFETs with Al₂O₃, AlN, Ta₂O₅, and TiO₂ barriers, respectively. The vertical-spin MOSFET can be modeled as a structure consisting of a symmetric FM/I/n-Si/I/FM multilayer [2,16] [see the inset of Fig. 1(a)], whose two-terminal MR ratio can be calculated according to the analytical equations of Fert and Jaffrès.9) Figure 4 presents the results of the MR ratio for vertical-spin MOSFETs with a moderate channel length, i.e., \( L_{N} = 100 \text{ nm} \). According to panels (a) to (d), we can compare the optimum parameter windows for the MR ratio of spin MOSFETs with Al₂O₃, AlN, Ta₂O₅, and TiO₂ barriers. For conventional barriers, such as Al₂O₃ and AlN, a MR ratio \( >2\% \) usually requires heavy doping with \( N_D > 10^{20} \text{ cm}^{-3} \) and an ultrathin barrier with \( d_{I} < 1 \text{ nm} \). These conditions are difficult to achieve experimentally, which is consistent with the obstacle revealed in previous studies.12,13) Figure 4(d) plots the proportion in FM contacts with low barriers, such as TiO₂ and Ta₂O₅, are orders of magnitude smaller than that of the conventional tunnel contacts. Therefore, the maximum MR signal and optimum parameter window for TiO₂ and Ta₂O₅ contacts are larger than those for the conventional tunnel contacts. Interestingly, we also demonstrate that the spin-asymmetry coefficient \( \gamma \) of the TiO₂ contact has a negative value, and the \( \gamma \) of the Ta₂O₅ contact can be tuned from negative to positive by changing the thickness of the tunnel barrier and the temperature. The optimized spin signals and unique spin-asymmetry properties of low-barrier tunnel contacts can be utilized for developing efficient spintronic devices.

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