Theory of in-plane current induced spin torque in metal/ferromagnet bilayers

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Abstract

Using a semiclassical approach that simultaneously incorporates the spin Hall effect (SHE), spin diffusion, quantum well states, and interface spin-orbit coupling (SOC), we address the interplay of these mechanisms as the origin of the spin–orbit torque (SOT) induced by in-plane currents, as observed in the normal metal/ferromagnetic metal bilayer thin films. Focusing on the bilayers with a ferromagnet much thinner than its spin diffusion length, such as Pt/Co with $\sim 10$ nm thickness, our approach addresses simultaneously the two contributions to the SOT, namely the spin-transfer torque (SHE-STT) due to SHE-induced spin injection, and the inverse spin Galvanic effect spin–orbit torque (ISGE-SOT) due to SOC-induced spin accumulation. The SOC produces an effective magnetic field at the interface, hence it modifies the angular momentum conservation expected for the SHE-STT. The SHE-induced spin voltage and the interface spin current are mutually dependent and, hence, are solved in a self-consistent manner. The result suggests that the SHE-STT and ISGE-SOT are of the same order of magnitude, and the spin transport mediated by the quantum well states may be an important mechanism for the experimentally observed rapid variation of the SOT with respect to the thickness of the ferromagnet.

Keywords: spin Hall effect, spin-transfer torque, spin–orbit torque, thin film spintronics, spin diffusion

(Some figures may appear in colour only in the online journal)

1. Introduction

Ever since the spin-transfer torque (STT) was proposed for the current perpendicular to the plane (CPP) geometry of magnetic heterostructures [1, 2], current induced spin torque has become a major topic in the spintronic research [3–6], as it demonstrates the feasibility of electrical control of magnetization dynamics. To improve the efficiency of magnetization switching, one often aims at reducing the volume or thickness of the magnetic component of the device, which generally enhances quantum effects on the magnetization dynamics, especially when the thickness of the heterostructures is reduced to the nanometer range. One particularly promising set of systems, owing to its simplicity in manufacturing, are normal metal/ferromagnetic metal (NM/FMM) bilayer thin films, each layer of thickness of a few nanometers, and the NM a heavy metal such as Pt or Ta [7–11]. The intriguing feature discovered in these thin films is that, in contrast to the CPP configuration, a spin torque, commonly referred to as the spin–orbit torque (SOT) [12], manifests itself in the current-in-plane (CIP) configuration, whose origin has been attributed to at least the following two mechanisms.

The first is the so-called inverse spin Galvanic effect spin–orbit torque (ISGE-SOT) originally proposed for a two dimensional system subject to the inversion symmetry breaking in the out-of-plane direction, in which Rashba spin–orbit coupling (SOC) is anticipated [12–18]. An in-plane current induces a spin accumulation in these systems, which then exerts a torque on the magnetization due to the exchange coupling between the conduction electron spin and the magnetization. The interface between NM and FMM obviously breaks the inversion symmetry, hence the ISGE-SOT is expected to occur in the CIP.
configuration. The second mechanism comes from the spin Hall effect (SHE) in the NM [19–23], in which an in-plane charge current causes a spin current in the transverse direction. This spin current causes a spin injection into the FMM, resulting in a spin torque. This contribution to the spin torque is frequently called spin Hall effect spin-transfer torque (SHE-STT).

On top of these two mechanisms, the seemingly simple NM/FMM bilayer in reality hosts a number of complexly intertwined features, including anisotropic magnetoresistance (AMR) [24], giant magnetoresistance (GMR)-like effects [25, 26], spin diffusion [27–29], quantum well states [30, 31], anomalous Hall effect (AHE) [32–34], Berry phase [21, 35], Edelstein effect [36], anisotropy field, Oersted field, as well as more practical issues such as magnetic domains, structural defects, and spin dependent scattering. A unified theory that can take into account all these effects to explain the observed SOT has yet to be formulated, and may be too complicated to analyze. Thus, attempts to devise a theoretical description for the SOT have been focusing on some of these mechanisms that are thought to be most relevant. Using different approaches, a damping-like spin torque is attributed to the combined effect of interface SOC and spin relaxation [37, 38] or spin dependent scattering [39]. A semiclassical theory that combines the drift-diffusion approach with the Boltzmann equation has also been proposed [40], from which the spatial profile of spin voltage under the influence of spin diffusion, SHE, and interface Rashba SOC are obtained. First principle calculations concerning SOT and realistic band structures have also been performed [41, 42]. The dependence of the SOT on the magnetization direction [11, 43] has been attributed to the anisotropic spin relaxation rates [44] and the Berry phase effect [45], and more sophisticated treatments of interface effects on the SOT based on magneto-electronic circuit theory [46], drift-diffusion model [47], and a fully three-dimensional perturbative approach [48] have also been proposed.

Here we present a semiclassical theory for the NM/FMM bilayer in the limit that the FMM is much thinner than its spin diffusion length. We consider this limit to be relevant to most experiments that use ferromagnetic materials whose bulk spin diffusion length exceeds the film thickness by far, such as Co and Ni, but not applicable to materials with short spin diffusion length such as permalloy [49]. Our treatment incorporates four of the aforementioned intertwined mechanisms and the appropriate theoretical methods to describe them, namely the spin diffusion equation for the SHE and spin diffusion in the NM [27–29], the quantum Boltzmann approach for the interface Rashba SOC [14, 18], and the quantum tunneling theory for the SHE induced spin injection mediated by the quantum well state [29, 50, 51]. Our goal is not to quantify the SOT for a specific set of bilayers, since we made several approximations to simplify our calculations, including the parabolic band and the sharp Rashba interface approximation. Rather, we aim at the behavior of generic bilayers considering how each material parameter influences the SHE-STT part and the ISGE-SOT part of the SOT, which may help to engineer the SOT for practical applications. We particularly focus on four of the system parameters, namely the FMM thickness $t_{\text{FMM}}$, NM thickness $t_{\text{NM}}$, exchange coupling $J_{\text{ex}}$, and interface SOC $\alpha_{\text{R}} k_F$, which one could control in real devices, and show how their interplay can explain a number of experimental observations, such as the rapid variation of the SOT with respect to the FMM thickness [52]. Although we limit our discussion to a single domain FMM, the two parts of the SOT are expected to contribute to the current induced domain wall motion observed in the NM/FMM bilayers where the FMM consists of multiple domains [53–55]. Hence, our discussion is also relevant to several phenomena therein, especially the dependence on the layer thickness.

In this article we treat the following points. In section 2, we formulate a quantum tunneling theory for the interface spin current, which is then combined with the spin diffusion equation to self-consistently solve for the interface spin voltage and the interface spin current. The SHE-STT and the issue of angular momentum conservation are then addressed. The ISGE-SOT is then calculated from the interface SOC, which joins the SHE-STT to give the total SOT. Numerical results using realistic parameters are then presented. Section 3 gives a summary of the features revealed by our approach.

2. Theoretical description of NM/FMM bilayer

2.1. Assumptions

We start with a brief discussion of the four key elements under consideration, namely the SHE, spin diffusion, quantum well states, and interface SOC, and the proper treatment for each of them, under the assumption that the spin transport is purely diffusive in the NM and purely quantum in the FMM. The SHE and spin diffusion in the NM have to be treated on equal footing by solving the spin diffusion equation [27]. In such a treatment, an important constraint is the spin current at the interface between NM and FMM, which serves as a boundary condition for the spin diffusion equation and hence affects the spatial profile of the spin voltage induced by SHE [28]. Previous theories treat the interface spin current as an external parameter, and adopt the value from first principle calculations or experimental results [28]. In contrast, it is our main goal to include the calculation of the interface spin current into a self-consistent microscopic theory that simultaneously addresses SHE, spin diffusion equation, and interface spin current.

Through the setup of such a self-consistent microscopic theory, we uncover several important aspects in this problem. First, since the spin transport in the FMM is purely quantum, it is mediated by the quantum well state wave function in the FMM [30, 31]. For this reason we employ the quantum tunneling theory for the interface spin current as a proper theoretical treatment [50]. Second, since the charge current flows in-plane but the spin injection is along out-of-plane direction, the SHE-induced nonequilibrium electrons presumably have both in-plane $k_x, y$ and out-of-plane $k_x, \hat{x}$ momentum. For the sake of investigating the interplay between $k_x$ and $k_y$, we focus on one particular component of the nonequilibrium electrons, namely the momentum in both directions are close to the Fermi momentum $k_F \approx k_y \sim k_x$. Third, the interface spin current calculated from the quantum tunneling theory turns out to depend on the spin voltage in the NM. On the other hand, the spin voltage also depends on the interface spin current
through the spin diffusion equation. Thus, the two have to be solved in an iterative manner. After the solutions are obtained, the interface spin current is identified with SHE-STT through angular momentum conservation [2, 50]. Remarkably, we find that the interface SOC modifies this angular momentum conservation, provided the nonequilibrium electrons have a finite in-plane momentum \(k_x\). This completes our treatment for the SHE-STT part of the SOT.

The last ingredient we incorporate is the interface Rashba SOC, whose origin lies in a variety of microscopic mechanisms such as SOC at the atomic level combined with the surface potential [56], the asymmetry of the wave function near the nucleus [57], rearrangement of atoms, etc, and in practice its range may extend over several atomic layers. The detailed microscopic origin and range of this SOC are not of our concern here. Rather, we focus on how interface SOC affects the nonequilibrium spin transport in the NM/FMM bilayer. To simplify the calculation, we employ the sharp-interface approximation [40] that assumes a \(\delta\)-function-like SOC confined to the interface \(\alpha = 0\), where the prefactor serves as a phenomenological fitting parameter. The interface SOC produces another contribution to the SOT, namely the ISGE-SOT, whose origin lies in a variety of microscopic mechanisms such as SOC at the atomic level combined with the surface potential [56], the asymmetry of the wave function near the nucleus [57], rearrangement of atoms, etc, and in practice its range may extend over several atomic layers. The detailed microscopic origin and range of this SOC are not of our concern here. Rather, we focus on how interface SOC affects the nonequilibrium spin transport in the NM/FMM bilayer. To simplify the calculation, we employ the sharp-interface approximation [40] that assumes a \(\delta\)-function-like SOC confined to the interface \(\alpha = 0\), where the prefactor serves as a phenomenological fitting parameter. The interface SOC produces another contribution to the SOT, namely the ISGE-SOT, whose origin lies in a variety of microscopic mechanisms such as SOC at the atomic level combined with the surface potential [56], the asymmetry of the wave function near the nucleus [57], rearrangement of atoms, etc, and in practice its range may extend over several atomic layers.

Before proceeding to our formalism, a proper definition of several technical terms mentioned above is in order. The spin voltage at position \(x\) in both NM and FMM is defined as the splitting between spin up and spin down local chemical potential \(\mu_x = (\mu_x^+ - \mu_x^-)\hat{\mu}_x\) polarized along the local spin quantization axis \(\hat{\mu}_x\). In contrast, the spin current \(j_x\) at position \(x\) is defined differently for the two layers. The existence of SOC and spin diffusion in the NM implies that the spin current is not conserved in the NM, \(\partial_x j_x + \partial_y (s)_y \neq 0\), where \((s)_y\) is the local electron spin density [58]. In addition, the contribution from SHE needs to be taken into account, leading to an expression that consists of the SHE spin current and the gradient of the spin current [27] (see equation (7)). On the other hand, since the FMM is free from spin diffusion, the spin current therein is conserved \(\partial_x j_x + \partial_y (s)_y = -\tau_x\) and is equal to the spin flux carried by the quantum state wave function [50] (see equation (5)), where \(\tau_x\) is the local spin torque. Consequently, one expects that the net spin current injected into the FMM, i.e. the interface spin current, is equal to the spin torque exerted on the magnetization. The identification of the interface spin current with the SHE-STT part of the spin torque is referred to as the angular momentum conservation [2, 50]. Finally, our approach is semiclassical in the sense that the momentum-out-of-plane direction is treated as a good quantum number, but the electron propagation is subject to the position-dependent spin voltage and exchange coupling to the magnetization.

2.2. Self-consistent treatment of spin voltage and SHE-STT

As discussed in section 2.1, we first introduce a semiclassical formalism that self-consistently addresses the spin voltage \(\mu_x\), spin current \(j_x\), and SHE-STT \(\tau_{\text{STT}}\). Our treatment is based on the assumption that the spin transport in the FMM is purely of quantum nature, since it is much thinner than its spin diffusion length \(\lambda \gg l_{\text{FM}}\). The spin transport in the NM is assumed to be purely diffusive, except near the interface \(x \lesssim 0\) where the spin voltage causes a spin injection that is described within the quantum tunneling formalism [50]. We define the out-of-plane direction to be \(\hat{x}\) and the direction of charge current to be \(\hat{y}\) [1, 29, 50, 51], as shown in figure 1, in contrast to the experimental convention of coordinates which are denoted by \((x', y', z')\). Owing to the translational invariance in the \(yz\)-plane, the spin voltage and the spin current are only functions of out-of-plane coordinate \(x\). As discussed in section 2.1, we assume the incident electron to have momentum both normal \(k_x\hat{x}\) and parallel \(k_y\hat{y}\) to the interface. To incorporate the translational invariance, we perform a separation of variables for the Hamiltonian and the wave function that describe the entire FMM and the NM near the interface

\[
H = \sum_{i=N,F} H_{i,x} + H_{i,yz},
\]

where \(\{N, I, F\}\) stands for NM, interface, and FMM, respectively. Within the parabolic band approximation, the out-of-plane component of the Hamiltonian is

\[
H_{N,x} = \frac{\hbar^2 k_x^2}{2m} - \frac{\mu_0 \cdot \sigma}{2} \quad (\text{for } x \lesssim 0),
\]

\[
H_{F,x} = \frac{\hbar^2 k_x^2}{2m} + J_{sd} \mathbf{S} \cdot \sigma \quad (0 \leq x \leq l_{\text{FM}}),
\]

\[
H_{I,x} = \alpha_{q}(k \times \hat{x}) \cdot \sigma \delta(x)a,
\]

Figure 1. Schematics of the NM/FMM bilayer. The quantum tunneling theory adopts the coordinate \((x, y, z)\) where out-of-plane direction is \(\hat{x}\), in contrast to the experimental coordinate \((x', y', z')\) where out-of-plane direction is denoted by \(\hat{z}'\). The FMM magnetization expressed in these coordinates is \(\mathbf{S} = (S_x, S_y, S_z) = S(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)\) and \(\mathbf{S} = (S_x', S_y', S_z') = S(\sin \theta' \cos \varphi', \sin \theta' \sin \varphi', \cos \theta')\). Blue arrows indicate the spatial profile of SHE induced spin voltage \(\mu_{i0}\) in the NM under the influence of spin diffusion and interface spin current \(j_{i0}\). The spin voltage at the interface is denoted by \(\mu_{i0} = \langle \mu(x')_i, \mu_y(x')_i \rangle = \langle \mu(x)_i | \sin \theta_0 \cos \varphi_0, \sin \theta_0 \sin \varphi_0, \cos \theta_0 \rangle\). The thickness of NM and FMM are labeled by \(l_{\text{NM}}\) and \(l_{\text{FM}}\), respectively, and the interface is located at \(x = 0\).
where we approximate the spin voltage on the NM side near the interface by its interface value $\mu_{S} \approx \mu_{0} = |\mu_{0}|(\cos \varphi \sin \theta_{1}, \sin \varphi \sin \theta_{1}, \cos \theta_{1})$. The spin voltage splits the degeneracy of spin $\sigma = \{ \uparrow, \downarrow \}$ quantized along $\mu_{0}$. The $J_{sd}$ is the exchange coupling between conduction electron spin and the magnetization $S = S(\cos \varphi \sin \theta, \sin \varphi \sin \theta, \cos \theta)$, which is set to be negative $J_{sd} < 0$ such that the conduction electron spin and the magnetization tend to be parallel. The $\alpha_{R}$ term is the fitting parameter to the Rashba SOC of any origin that gives the form in equation (2), assumed to be sharply confined at the interface [41], and the $\beta_{R}$-function is multiplied by Fermi wave length $a$ to keep track of the dimension. We stress that this sharp interface approximation is merely for the sake of simplifying the calculation and modeling the generic situation of inversion symmetry breaking. A more sophisticated treatment of the interface SOC is not expected to modify the statements obtained from this approximation. The corresponding wave functions in the out-of-plane direction are

$$
\psi_{N}(x) = (Ae^{i\phi_{x}} + Bc^{-i\phi_{x}}) \left( e^{i\frac{\nu}{2} \cos \theta} \frac{e^{i\frac{\nu}{2} \sin \theta}}{2} \right) + Ce^{-i\phi_{x}} \left( -e^{i\frac{\nu}{2} \sin \theta} \frac{e^{i\frac{\nu}{2} \cos \theta}}{2} \right),
$$

$$
\psi_{F}(x) = e^{i\phi_{x}} \left[ k_{F}(x - l_{FM}) \right] D \left( e^{i\frac{\nu}{2} \cos \theta} \frac{e^{i\frac{\nu}{2} \sin \theta}}{2} \right) + e^{-i\phi_{x}} \left[ k_{F}(x - l_{FM}) \right] E \left( -e^{i\frac{\nu}{2} \sin \theta} \frac{e^{i\frac{\nu}{2} \cos \theta}}{2} \right),
$$

where the spinor of $\psi_{N}$ and $\psi_{F}$ are quantized along the interface spin voltage polarization and the magnetization, respectively. Recent angle-resolved photoemission spectroscopy experiments in NM/FMM bilayers unambiguously demonstrate the existence of the exchange-split quantum well states [30, 31], which is described by the oscillatory wave function $\psi$ in our formalism. The wave function outside of the FMM $x > l_{FM}$, which is usually an oxide insulator or vacuum, is assumed to vanish for simplicity [29].

The spin voltage is caused by the nonequilibrium electrons that also have momentum $k_{y}$ $k_{y} \approx k_{F} y$, since the charge current is flowing along $y$ direction. Thus the Rashba term reads $H_{R} = -\alpha_{R} k_{y} \sigma_{x} \delta(x)a$. Defining $\beta_{R} = 2\alpha_{R} k_{y} e^{2}/\hbar^{2}$, the matching conditions at the interface is affected by the interface SHE [59]

$$
\psi_{F}(0) - \psi_{N}(0) = 0,
$$

$$
\partial_{x} \psi_{F}(x)|_{x=0} - \partial_{x} \psi_{N}(x)|_{x=0} = \beta_{R} \sigma_{y} \psi_{N/F}(0),
$$

(4)

which are used to solve the coefficients $B \sim E$ in terms of the incident amplitude $A$, as detailed in Appendix A. The incoming flux is then identified with the interface spin voltage by $|A|^{2} = N_{F} |\mu_{0}| / a^{3}$, where $N_{F}$ is the density of states per $a^{3}$. This identification bridges the quantum tunneling formalism above and the spin diffusion equation below. The incoming flux $|A|^{2} = N_{F} |\mu_{0}| / a^{3}$ of the plane wave is proportional to the magnitude of the charge current flowing in $y$-direction, but $J_{sd}$ and $\beta_{R}$ are material properties independent of the charge current.

The interface SOC renders an interesting consequence for the angular momentum conservation [2]. The spin current right before $(x = 0-)$ and right after $(x = 0+)$ the interface is, using equation (4),

$$
\begin{align*}
J_{0-} &= \frac{h}{4\sin} \left[ \psi_{N/F}^{*} \sigma_{y} \partial_{x} \psi_{N/F} \right]_{x=0} - \left( \partial_{x} \psi_{N/F}^{*} \sigma_{y} \psi_{N/F} \right)_{x=0} \\
&= \frac{h}{4\sin} \left[ \psi_{N/F}^{*} \sigma_{y} \partial_{x} \psi_{N/F} \right]_{x=0} - \left( \partial_{x} \psi_{N/F}^{*} \sigma_{y} \psi_{N/F} \right)_{x=0} \\
&- \beta_{R} \psi_{N/F}^{*} \left( \sigma_{y} \sigma_{z} - \sigma_{z} \sigma_{y} \right) \psi_{N/F} \\
&= J_{0+} + \delta_{y},
\end{align*}
$$

(5)

That is, in the presence of interface SOC, the spin current is not conserved across the interface. Evidently, this is because the SOC effectively acts like a magnetic field at $x = 0$, hence changing the polarization of the injected spin current. The discontinuity of spin current in the presence of SOC, with the effect of spin memory loss incorporated, has also been reported based on a first principle calculation [60]. The spin–orbit filtering and spin–orbit precession, which are not incorporated in our theory, have also been shown to lead to the discontinuity of spin current [46, 47, 61].

One may further calculate the spin accumulation at position $x$ inside the FMM by $(\sigma_{x}) = \psi_{F}^{*}(x) \sigma_{x} \psi_{F}(x)$, and then multiply by cross section unit and integrate along out-of-plane direction to get the total spin accumulation $(\overline{\sigma} = a^{2} \int_{0}^{l_{FM}} \sigma_{x} \, dx)$. The SHE-STT is then obtained via Landau–Lifshitz dynamics, and we find that

$$
\tau_{STT} = \frac{J_{sd}}{\hbar} \overline{\sigma} \times S = a^{2} J_{0+},
$$

(6)

meaning that the SHE-STT is equal to the spin current right after the interface $J_{0+}$ but not before $J_{0-}$. This feature is not included in our previous treatments [29, 50, 51]. Comparing equations (5) and (6), we see that interface SOC changes angular momentum transferred from the NM to FMM, thus engineering interface SOC may also influence the SHE-STT.

We proceed to review the spin diffusion approach that describes the spin voltage in the NM [27, 62], and how the interface spin current modifies the landscape of the spin voltage [28]. The quantum tunneling theory from equations (3) to (5) will be incorporated into this diffusive formalism later. The spin diffusion approach is based on the following properties of the NM: (a) The spin current in NM consists of both the spatial gradient of spin voltage and the bare SHE spin current $j_{SH}^{\text{STT}} = \sigma_{c} e / 2 e$, i.e.

$$
\begin{align*}
\delta j_{c} &= - \frac{\sigma_{c}}{4e^{2}} \partial_{x} \mu_{x} + j_{SH} \hat{e},
\end{align*}
$$

(7)

where $\sigma_{c}$ is spin Hall angle, $\sigma_{c}$ is the conductivity of NM, $E = j_{c} / \sigma_{c}$ is the electric field in $y$ direction, and $-e$ is electron charge. (b) The spin voltage obeys the spin diffusion
\[ \nabla^2 \mu_s = \mu_s / \lambda^2, \] where \( \lambda \) is the spin diffusion length, and hence has a general solution

\[ \mu_s = Ae^{i\pi/\lambda} + Be^{-i\pi/\lambda}. \] (8)

(c) Spin current vanishes at the edge of NM, \( j_{\text{in}} = 0 \), which serves as one boundary condition. (d) The spin current at the interface is described by the \( j_{\text{in}} \) in equation (5), i.e. the spin current at the interface, which serves as another boundary condition. The self-consistent solution satisfying (1)–(4) gives the landscape of the spin voltage and the spin current [28]

\[ \mu_s = \tilde{\mu}_0 \frac{\sinh (\frac{2\lambda + k\lambda}{2\lambda})}{\sinh (\frac{k\lambda}{2\lambda})} \tilde{z} - \frac{4e^2\lambda}{\sigma_e} \frac{\cosh (\frac{2\lambda + k\lambda}{2\lambda})}{\sinh (\frac{k\lambda}{2\lambda})} j_{\text{in}} - \frac{\sigma_e}{2e^2\lambda} \frac{\cosh (\frac{2\lambda + k\lambda}{2\lambda})}{\sinh (\frac{k\lambda}{2\lambda})} j_{\text{in}}, \] (9)

where \( \tilde{\mu}_0 = 2e\lambda\theta_{\text{SH}}E \tanh (h/N/2\lambda) \) is the surface spin voltage when the NM is not attached to the FMM. Equations (7)–(9) remain valid even in the presence of SOC, as they only rely on the assumptions (a)–(d) which remain true even in the presence of SOC.

Exactly at the interface, the spin voltage satisfies

\[ \mu_s = \tilde{\mu}_0 \frac{\sinh (\frac{2\lambda + k\lambda}{2\lambda})}{\sinh (\frac{k\lambda}{2\lambda})} \tilde{z} + \frac{2e^2\lambda}{\sigma_e} \frac{\sinh (\frac{2\lambda + k\lambda}{2\lambda})}{\sinh (\frac{k\lambda}{2\lambda})} j_{\text{in}} - \frac{\sigma_e}{2e^2\lambda} \frac{\sinh (\frac{2\lambda + k\lambda}{2\lambda})}{\sinh (\frac{k\lambda}{2\lambda})} j_{\text{in}} - \frac{4e^2\lambda}{\sigma_e} \frac{\cosh (\frac{2\lambda + k\lambda}{2\lambda})}{\sinh (\frac{k\lambda}{2\lambda})} j_{\text{in}}. \] (10)

so the interface spin voltage is determined by the interface spin current. 

The expression inside the bracket is usually of the order of unity. Thus, the STT alone is in the range of GHz, consistent with that measured experimentally.

### Table 1. Summary of the notations and their order of magnitude values when the external charge current is fixed at \( j_e \sim 10^{13} \text{A m}^{-2} \).

| Parameter | Value |
|-----------|-------|
| Fermi momentum | \( k_F \sim 1/\alpha \text{nm}^{-1} \) |
| Fermi energy | \( e\phi \sim \text{eV} \) |
| Conductivity | \( \sigma_e \sim 10^7 \text{S m}^{-1} \) |
| Spin Hall angle | \( \theta_{\text{SH}} \sim 0.1 \) |
| NM spin diffusion length | \( \lambda \sim 10 \text{nm} \) |
| External charge current | \( j_e \sim 10^{13} \text{A m}^{-2} \) |
| External field | \( E \sim 10^7 \text{mkg Cs}^{-2} \) |
| Relaxation time | \( \tau \sim 10^{-14} \text{s} \) |
| Dimensionless magnetization | \( S \sim 1 \) |
| Bare spin Hall spin current | \( j_{\text{SH}} \sim 10^{29} \text{m}^{-3} \) |
| Temperature in ISGE-SOT integral | \( k_B T \sim 0.02 e\phi \) |

#### 2.3. SOC induced spin accumulation and ISGE-SOT

We proceed to address the other component of the SOT, namely the ISGE-SOT [14, 15, 17, 18, 39, 41]. From equation (1), we isolate the \( yz \) plane at \( x = 0 \) and consider the Hamiltonian

\[ H_{\text{yz}} = \delta(x) a \frac{h^2 (k_x^2 + k_y^2)}{2m} + \left[ \alpha_B (k \times \hat{x}) + J_{\text{sd}} S - \frac{\mu_0}{2} \cdot \sigma \right], \] (14)

where \( k = (0, k^x, k^y) = k(0, \cos \xi, \sin \xi) \) is the in-plane momentum. Equation (14) describes an interface simultaneously under the influence of interface Rashba SOC, exchange coupling, and the interface spin voltage since it is a inversion symmetry breaking interface proximity to both the NM and the FMM. However, using the typical values for the parameters in table 1, the interface spin voltage is typically \( |\mu_0| \sim 10^{-5} \text{eV} \), which is few orders of magnitude smaller than the SOC \( \alpha_B k^2 \sim 0.01 \text{eV} \) and the exchange coupling \( J_{\text{sd}} \sim 0.1 \text{eV} \), meaning that interface spin voltage is not crucial for the ISGE-SOT. In the calculation below we ignore the \( \mu_0 \) term in equation (14) for simplicity. This also means that ISGE-SOT is not influenced by the self-consistent approach to SHE-STT in section 2.2.

Our aim is to calculate the spin accumulation induced by an in-plane current flowing along \( y \) direction using quantum Boltzmann equation. Assuming the relaxation time \( \tau \) is the same for the two bands of the Hamiltonian, denoting \( j_{\text{in}}^0 \) as the equilibrium Fermi distribution for the two bands, and \( \mathbf{E} = \mathbf{E}^f \) as the electric field associated with the charge current, the leading order distribution function is

\[ g_{k,\pm} = -\frac{e}{h} \mathbf{E} \cdot \mathbf{v}_{k,\pm} \frac{\partial f_{k,\pm}^0}{\partial E_{k,\pm}}. \] (15)

from which one calculates the interface spin accumulation via the Boltzmann equation

\[ \left\langle \delta \sigma \right\rangle_{\pm} = \int \frac{\partial \mathbf{k}}{(2\pi/\alpha)^2} \left( \sigma \right)_{\pm} g_{k,\pm}. \] (16)
where we denote the spin expectation value of the eigenstate as $\langle \sigma \rangle _{\pm}$. In appendix B, we provide a formalism that is convenient for numerically calculating $\langle \delta \sigma \rangle _{\pm}$ at any values of $\{\alpha k_{F}, J_{sd}\}$. The total spin accumulation is the sum of the contribution from each band $\langle \delta \sigma \rangle = \langle \delta \sigma \rangle _{+} + \langle \delta \sigma \rangle _{-}$, which is multiplied by lattice unit area and $\delta(x)\,a$ due to equation (14) and then integrated along out-of-plane direction to get the total spin accumulation in the whole FMM film $\langle \delta \sigma \rangle = a^2 \int_{0}^{L} dx \langle \delta \sigma \rangle \delta(x)\,a = a^2 \langle \delta \sigma \rangle$. The ISGE-SOT then follows from the Landau–Lifshitz dynamics

$$\tau_{ISGE} = \frac{J_{sd}}{\hbar} \langle \delta \sigma \rangle \times \mathbf{S}. \quad (17)$$

Since $\tau_{ISGE}$ comes from the interface SOC, it does not strongly depend on the FMM thickness. From equation (B.6), we see that it is convenient to introduce a frequency scale

$$\omega _{1} = \frac{3/2}{\epsilon F\sqrt{2m}} \frac{\sqrt{2m}}{4\pi \hbar a} \sim 10 \text{ GHz}, \quad \frac{\hbar \omega _{1}}{\mu _{B}} \sim 100 \text{ mT}, \quad (18)$$

after using the typical values in table 1, and express ISGE-SOT accordingly

$$\tau_{ISGE} = \left( \frac{J_{sd}}{\epsilon F} \right) \omega _{1} \mathbf{I} \times \mathbf{S}, \quad (19)$$

where $\mathbf{I}$ is the dimensionless integral part of equation (B.6) whose numerical value is typically of the order of unity. Comparing equations (12) and (18), one sees that SHE-STT and ISGE-SOT have comparable magnitudes, and both are in the GHz regime, in accordance with that measured experimentally.

### 2.4. Numerical results

Following the experimental convention, we define the field-like $\mathbf{S} \times \mathbf{z}$ and damping-like $\mathbf{S} \times (\mathbf{S} \times \mathbf{z})$ direction from $\mathbf{z}$ and $\mathbf{S}$. Note that they are different from that defined from $\mathbf{\mu }_{d}$ and $\mathbf{S} [29, 50, 51]$. The total SOT, i.e. the sum of the SHE-STT discussed in section 2.2 and the ISGE-SOT discussed in section 2.3, is then projected into these two components

$$\tau = \frac{d\mathbf{S}}{dt} = \tau_{STT} + \tau_{ISGE}$$

$$= \tau _{F} \mathbf{S} \times \dot{\mathbf{z}} + \tau _{d} \mathbf{S} \times (\mathbf{S} \times \dot{\mathbf{z}}). \quad (20)$$

Below we discuss the numerical result of $\mathbf{\mu }_{d}$ and $\mathbf{j}_{d}$ as well as the dependence of $\tau _{F}$ and $\tau _{d}$ on various material parameters.

Figure 2 shows the spatial profile of $\mathbf{\mu }_{d}$ and $\mathbf{j}_{d}$ for several different system parameters, after substituting the $\mathbf{\mu }_{0}$ and $\mathbf{j}_{0}$-solved self-consistently from equation (11) into equation (9). On the FMM side, we convert the spin expectation value $\langle \sigma _{\gamma} \rangle$ into a spin voltage by $\mathbf{\mu }_{d} = a^2 \langle \sigma _{\gamma} \rangle /N_{\gamma}$ such that the spatial profile of the spin voltage in the entire NM/FMM bilayer can be investigated. The local spin current is calculated from the spin diffusion equation [27, 28], whereas in the FMM it shows clear features of oscillation due to the quantum well state described by the $\psi _{F}$ in equation (3). The precise shape of $\mathbf{\mu }_{d}$ in the FMM is a combined effect of quantum interference of the spin transport [29, 50] and the self-consistency of equation (11), and varies significantly with $k_{F}$ and $J_{sd}$, as can be seen by comparing plots with different parameters in figure 2. The spin voltage is not continuous across the interface, a result of treating the NM as purely diffusive and the FMM as purely quantum. Rather, the conserved quantity is the spin current according to equation (5) is taken into account. As expected, the bigger is the SOC, the more discontinuous is the spin current at the interface, as can be seen by comparing figures 2(b) and (d).

![Figure 2](image)

Figures 3(a) and (b) shows the thickness dependence of $\tau _{F}$ and $\tau _{d}$. As a function of the FMM thickness $l_{FM}$, both components show a dramatic oscillatory dependence, again due to the spin transport mediated by the quantum well state, which seems to coincide with the experimentally observed rapid variation of the SOT [52] at least in some reasonable parameter regime. The oscillatory behavior also sensitively depends on the exchange coupling $J_{sd}$. Exceeding a certain FMM thickness, the SOT may change sign. As a function of NM thickness $l_{N}$, both components increase smoothly in the regime $l_{N} \sim \lambda$, owing to the fact that the interface spin voltage $\mathbf{\mu }_{d}$ generally increases with $l_{N}$ in this regime, causing an increase in the spin injection and hence the SOT. Note that the SOT...
may change sign with increasing $l_{NM}$, which can be a possible mechanism for the reversed domain wall motion observed in Pt/Co/Pt trilayer [63] with changing Pt thickness (although the quantum interference effect in the trilayer may be even more complicated). The above features all come from the SHE-STT part of the SOT but not the ISGE-SOT part, since in our sharp interface approximation the SOT is strictly confined to the interface and does not vary with either $l_{BF}$ or $l_{FM}$. The absolute magnitude of the SOT at current density $j_{c} \sim 10^{11}$ A m$^{-2}$, after converting to the effective field, is of the order of few tenths of $\hbar \omega_{0}/\mu_{B} \sim 100$ mT, close to that observed experimentally [7, 8, 11].

The SOT also shows clear modulations with the exchange coupling $J_{sd}$, as can be seen in figure 3(c). The oscillatory behavior with respect to both $l_{FM}$ and $J_{sd}$ points to a simple physical picture for how the spin transport mediated by quantum well state yields the SHE-STT: The conduction electron spin injected from the NM precesses around the magnetization when it travels inside the FMM. The phase difference between the injected and the reflected spin yields the SHE-STT. The phase difference is determined by how fast the spin precesses ($J_{sd}/\hbar$) and how much distance it travels ($l_{FM}$), hence the oscillatory behavior with respect to both $J_{sd}$ and $l_{FM}$. We remark that the ISGE-SOT part also depends on $J_{sd}$ since it enters the Boltzmann equation of calculating the spin accumulation, yet the dependence is rather smooth, so the rapid variations mainly come from the SHE-STT part. Our result indicates that, even in a clean FMM without other complications like domains or impurities, the quantum tunneling alone can already account for the rapid variation of the SOT [52]. Without invoking other mechanisms such as spin relaxation [37, 38] or spin dependent scattering [39], the ISGE-SOT alone is predominantly field-like at any $(J_{sd}, \alpha_{R}k_{F})$, thus the damping-like components in figures 3(a)–(d) are almost entirely contributed from the SHE-STT.

We now comment on how this thickness dependence relies on the assumptions made in our approach. As mentioned in sections 2.1 and 2.2, only one component of the nonequilibrium electrons $k_{x} \hat{x} + k_{y} \hat{y} \sim k_{F} \hat{x} + k_{F} \hat{y}$ is considered, whereas in realistic thin films the spin injection may come from all incident angles, and certain averaging over the Fermi surface should be performed. While averaging over the Fermi surface is expected to influence the quantum interference effect and mitigate the thickness dependence, further investigation that incorporates a microscopic theory of SHE is required to clarify how the averaging over Fermi surface should be done for the nonequilibrium spin injection, since the electric field is applied along $\hat{y}$ but the net spin injection is along $\hat{x}$. Nevertheless, we emphasize that through examining this single component $k_{x} \hat{x} + k_{y} \hat{y}$ we already uncover new features in this problem, including the mutual dependence between $J_{sd}$ and $\mu_{q}$ described by equation (11), and quantum interference effect mediated by the quantum well state, which should not be omitted in explaining the thickness dependence of the SOT.

Finally, we remark on the dependence of the SOT on the direction of the magnetization. Figure 4 shows $\tau_{j}$ and $\tau_{d}$ versus the angle $(\theta', \varphi')$ defined in the experimental coordinate (see figure 1). We use $(\theta', \varphi')$ such that comparison with experiments can be easily made [11, 43]. The torques are smallest when the magnetization points in-plane and perpendicular to the charge current, as indicated by the blue regions in figure 4, and increases when the magnetization moves away from this direction. These results are, however, at odds with those revealed by experiments, which concluded that the torque is larger when the magnetization has more in-plane components [11, 43]. Based on these results, we speculate that the mechanisms not taken into account by our treatment, such as the Berry phase effect [45] or anisotropic spin relaxation
rate [44], may be crucial to explain the angular dependence revealed by experiments.

3. Conclusions

In summary, using a semiclassical approach that simultaneously incorporates SHE, spin diffusion, quantum well state, and interface SOC, we address the in-plane current induced SOT in NM/FMM bilayers. Treating the NM as purely diffusive and the FMM as purely quantum, as considered relevant to most of the experiments, the approach reveals the following intriguing features. First, from the spin diffusion equation one sees that the spatial profile of SHE induced spin voltage is determined by the interface spin current [28], yet the interface spin current in turn also depends on the spin voltage. Thus, the two have to be solved in a self-consistent manner. Second, once the interface spin current is determined, one may naively identify it with the SHE-STT according to the angular momentum conservation [2]. The interface SOC, however, yields an effective interface magnetic field that alters this direct identification, and the interface spin current is equal to the SHE-STT only after the contribution from SOC is subtracted.

Third, although the interface spin voltage depends on the thickness of NM and FMM, it is a very small energy scale that practically does not influence the ISGE-SOT, hence the ISGE-SOT is independent from the thickness of the NM and the FMM. On the other hand, owing to the quantum interference effect of the injected conduction electron, the SHE-STT strongly depends on and may change sign with the thickness of the NM and the FMM, in accordance with the experimentally observed rapid variation of the SOT [52] and the sign change of current-induced domain wall motion [63] with respect to the layer thickness. Finally, using the parameters relevant to realistic thin films, the SHE-STT and ISGE-SOT are revealed to be of the same order of magnitude (∼GHz), comparable to that unveiled by experiments. Besides helping to understand the role of these complicated intertwined ingredients, we anticipate that our approach can help to guide the engineering of the SOT, whether one aims at changing the magnitude of the SOT or the relative weighting between its damping-like and field-like components.

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Appendix A. Tunneling amplitudes

Upon matching the boundary conditions in equation (4), and use the short-hand notation

$$\mu_1 = e^{-i\phi/2} \cos \frac{\theta_0}{4}, \quad \mu_2 = e^{i\phi/2} \sin \frac{\theta_0}{4},$$
$$\mu_3 = -e^{-i\phi/2} \sin \frac{\theta_0}{4}, \quad \mu_4 = e^{i\phi/2} \cos \frac{\theta_0}{4},$$
$$s_1 = e^{-i\phi/2} \cos \frac{\theta_0}{2}, \quad s_2 = e^{i\phi/2} \sin \frac{\theta_0}{2},$$
$$s_3 = -e^{-i\phi/2} \sin \frac{\theta_0}{2}, \quad s_4 = e^{i\phi/2} \cos \frac{\theta_0}{2},$$
$$\lambda_{\alpha\sigma} = i k_{\alpha} \left( 1 + e^{2ik_{\alpha}b_m} \right) + (ik_{0\alpha} + \gamma_{\alpha}\beta_{\alpha}) \left( 1 - e^{2ik_{\alpha}b_m} \right),$$
$$\xi = (\lambda_{+\downarrow} - s_1 s_2 \mu_3) / (\lambda_{-\downarrow} + s_4 \mu_1 - \lambda_{-\downarrow} - s_3 \mu_2),$$
$$\Omega = \lambda_{+\uparrow} + s_1 s_2 \mu_3 - \lambda_{+\downarrow} - s_4 \mu_1 \xi - \lambda_{+\uparrow} + s_3 \mu_2 - \lambda_{-\uparrow} - s_4 \mu_3 \xi,$$
$$\Omega = \lambda_{+\uparrow} + s_1 s_2 \mu_3 + \lambda_{-\uparrow} - s_4 \mu_1 \xi - \lambda_{+\uparrow} - s_3 \mu_2 - \lambda_{-\uparrow} - s_4 \mu_3 \xi,$$

(A.1)

where \( \{ \alpha, \gamma \} = \{ +, - \} \) and \( \sigma = \{ \uparrow, \downarrow \} \), the scattering coefficients are

$$B \frac{\Lambda}{A} = \frac{k_{0\uparrow} - k_{0\downarrow}}{k_{0\uparrow} + k_{0\downarrow}} - \frac{2k_{0\uparrow} (\mu_1 \mu_4 - \mu_2 \mu_3)(\lambda_{+\downarrow} - s_3 \xi)}{(k_{0\uparrow} - k_{0\downarrow}) \Omega \mu_1},$$
$$C \frac{\Lambda}{A} = \frac{2k_{0\uparrow} \Omega}{(k_{0\uparrow} - k_{0\downarrow}) \Omega},$$
$$D \frac{\Lambda}{A} = 2ik_{0\uparrow} \left( \mu_1 \mu_4 - \mu_2 \mu_3 \right), \quad E = \xi D.$$

(A.2)

The calculation of spin expectation values and the spin current are then straightforward as described in section 2.2.

Appendix B. Details of calculating the spin accumulation due to SOC

We provide a formalism that is convenient for numerically calculating the SOC induced spin accumulation in the parabolic band approximation at any \( \{ \alpha, \gamma, F_{sd} \} \). The Rashba SOC and exchange coupling in equation (14) together constitute an
effective, momentum dependent magnetic field in the interface Hamiltonian \(H_{3\gamma} = \hbar^2 k^2/2m + B_k \cdot \mathbf{\sigma} \), with
\[
\begin{pmatrix}
B_k^1 \\
B_k^2 \\
B_k^2
\end{pmatrix} = \begin{pmatrix}
J_{sd} S \sin \theta \cos \varphi \\
J_{sd} S \sin \theta \sin \varphi + \alpha_k k^2 \\
J_{sd} S \cos \theta - \alpha_k \kappa^2
\end{pmatrix},
\]
and hence the eigenvalues
\[
E_{k,\pm} = \frac{\hbar^2 k^2}{2m} \pm |B_k|.
\]
Defining the planar coordinate \( r = (0, y, z) \), the eigenstates are
\[
\psi_{\pm}(y, z) = \frac{e^{i k y}}{a^{3/2}} \left( B_k^0 \pm |B_k| \right) \left( B_k^0 \pm B_k^2 \right)
\]
where we define \( B_k = B_k^0 - i B_k^2 \). Consequently, the \( \alpha \)-component spin expectation value of the eigenstate is
\[
\langle \sigma^\alpha \rangle \pm = \psi_{\pm}^* (y, z) \sigma^\alpha \psi_{\pm} (y, z) = \pm |B_k|/|B_k|^3.
\]
The spin accumulation is then, by expressing equation (16) in polar coordinate,
\[
\langle \sigma \rangle \pm = \frac{\hbar^2 e^2}{4 \pi^2 \hbar} \int k \, dk \, d\xi \langle \sigma \rangle \pm
\]
Numerically, by defining the square root \( q \) of various energy scales
\[
\frac{\hbar^2 k^2}{2m} = q^2, \quad \frac{\hbar^2 k^2}{2m} = q^2, \quad k_{th} T = q^2 T,
\]
\[
\alpha_k k = q, \quad J_{sd} S = q^2 < 0,
\]
\[
|B_k| = \left[ q_1^2 + \frac{\alpha_k^2 q^2}{|B_k|} + 2q y q_j^2 \sin \theta \sin \varphi \sin \xi - \cos \theta \cos \xi \right]^{1/2},
\]
we can evaluate the integral at any \( \alpha_k k, J_{sd}, \theta, \varphi \) by explicitly calculating
\[
\langle \sigma \rangle \pm = \left( \frac{e}{4 \pi^2 \hbar a} \tau E \sqrt{2m/\hbar} \right) \int q \, dq \, d\xi
\]
For all the simulation presented in section 2.4, we fix the temperature at \( k_{th} T/\chi = 0.02 \). For any \( \alpha k, k_{sd}, \langle \sigma \rangle \pm \) is even under the inversion of magnetization \( S \rightarrow -S \), in agreement with several analytical limits reported previously [18, 64]. This can be seen by noting that the integral of equation (B.6) is invariant under \( \{ S^1, S^2, S^3 \} \rightarrow \{ -S^1, -S^2, -S^3 \} \) and a shift in the angular argument \( \xi \rightarrow \pi + \xi \).

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