Direct and inverse spin-orbit torques

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In collinear magnets lacking inversion symmetry application of electric currents induces torques on the magnetization and conversely magnetization dynamics induces electric currents. The two effects, which both rely on spin-orbit interaction, are reciprocal to each other. Revisiting the phenomenological modelling of the two phenomena, denoted direct and inverse spin-orbit torque, in light of their reciprocity, we show that the mere existence of the spin Hall effect (SHE) requires spin currents to decay spatially in materials with nonzero normal resistivity irrespective of the scattering mechanism underlying the resistivity. This SHE-mediated spin relaxation mechanism adds to the usual spin flip scattering induced spin relaxation mechanisms. Measurements of the direct spin-orbit torque (SOT) can be used to predict the inverse spin-orbit torque (ISOT), which is discussed for the case of currents induced under ferromagnetic resonance in magnetic bilayers. Based on the first principles density-functional theory framework we investigate SOT and ISOT in Co/Pt(111) magnetic bilayers within the Kubo linear response formalism. Spin and charge currents as well as torques are resolved on the atomic scale in order to expose the mechanisms underlying SOT and ISOT and to highlight their reciprocity on the microscopic level.

I. INTRODUCTION

In ferromagnetic materials Faraday’s law of induction needs to be generalized to include so-called spinmotive forces, i.e., electric fields induced by the magnetization dynamics. The spinmotive force can be interpreted as the reciprocal of the current-induced torque: A moving domain wall induces a spinmotive force and conversely an applied current drives domain wall motion. Thus, the electric fields induced by magnetization dynamics generate a feedback effect on the magnetization via the current-induced torques which they produce.

Spinmotive forces do not only occur in noncollinear magnetic structures such as domain-walls but can also in collinear magnets due to the interplay of spin orbit interaction with bulk or structural inversion asymmetry. Spin-orbit torques (SOTs), i.e., current-induced torques originating from spin orbit interaction in inversion asymmetric collinear magnets, are the reciprocal to the electric fields induced by magnetization dynamics in collinear magnets. Thus, we will denote the latter as inverse spin-orbit torques (ISOTs) in the following. ISOTs constitute a special case of spinmotive forces.

While earlier experiments on SOTs estimated the current-induced torques indirectly from the onset of nucleation of reversed domains or magnetization switching at critical current densities, direct measurements of SOTs have been performed recently in bilayer systems and the SOT has been determined as a function of magnetization direction. Two qualitatively different SOT components are found in these experiments on bilayer systems, the first one is an even function of \( \mathbf{M} \), the second one is an odd function. Denoting the applied in-plane electric field by \( \mathbf{E} \) and the unit vector in the out-of-plane direction by \( \hat{e} \), they are given by \( T^{\text{even}} = T^{\text{even}} \mathbf{M} \times ( [ \hat{e} \times \mathbf{E} ] \times \mathbf{M} ) \) and \( T^{\text{odd}} = T^{\text{odd}} ( \hat{e} \times \mathbf{E} ) \times \mathbf{M} \) to lowest order in \( \mathbf{M} \).

In bilayer systems based on 5d transition metals with large spin Hall effect (SHE), such as AlO\(_x\)/Co/Pt, MgO/CoFeB/Ta and CoFeB/W, the dominant contribution to \( T^{\text{even}} \) arises from the SHE\(^{13,14,18-22}\). Conversely, in Ni\(_{80}\)Fe\(_{20}\)/Pt the spin current pumped into Pt by exciting the ferromagnetic resonance (FMR) of Ni\(_{80}\)Fe\(_{20}\) induces an electric field via the inverse spin Hall effect (ISHE)\(^{23-25}\). Theoretically, an additional ISOT is expected from the Rashba spin orbit interaction at the bilayer interface. This theoretical prediction, that the ISOT in bilayer systems should not arise purely from the combination of spin pumping and ISHE, is supported by the experimental observation that for the reciprocal phenomenon, the SOT, \( T^{\text{odd}} \), can be as large as or even larger than \( T^{\text{even}} \).

So far only the dc voltage due to FMR-driven ISOT has been studied intensively in bilayer systems. However, after the theoretical prediction\(^{26}\) that the ac component is expected to be much larger than the dc one, several recent experiments have been devoted to its measurement\(^{21,31-33}\). As will be discussed in this work it is expected from the reciprocity of ISOT and SOT that the dc voltage generated by the FMR-driven ISOT is proportional to \( T^{\text{even}} \), while the ac voltage is determined by both \( T^{\text{even}} \) and \( T^{\text{odd}} \). Since the ac voltages associated with \( T^{\text{even}} \) and \( T^{\text{odd}} \) exhibit a phase difference of \( \pm 90^\circ \), a non-trivial phase relationship between ac signal and magnetization trajectory is expected. Phase-sensitive measurements of the ac ISOT-signal induced under FMR can thus be complementary to experiments on the SOT phenomenon. Both types of experiments, i.e., measuring the induced voltage under FMR on the one hand and measuring on the other hand the current-induced torque on the magnetization, can thus serve to determine \( T^{\text{even}} \) and \( T^{\text{odd}} \) and from them the parameters needed to model them, notably spin-diffusion length, spin-mixing conductance, SHE-angle as well as Rashba and Dresselhaus parameters.

This article is organized as follows: In section II we discuss the Kubo formalism expressions for both SOT and ISOT. In the case of the SOT phenomenon, the torque on the magnetization is given by \( \mathbf{T} = \mathbf{tE} \), which defines the torkance tensor
II. RELATIONSHIP BETWEEN DIRECT SOT AND INVERSE SOT

Reciprocity between current-induced torques and spinmotive forces has been discussed in detail in the framework of phenomenological modelling in this section. In this section, we revisit this reciprocity on the basis of the Kubo linear response formalism, which is well-suited to study SOT and ISOT from first principles. We consider a Hamiltonian of the form

$$H(r, t) = H_0(r) - m \cdot \dot{r}(t) \Omega^{xc}(r),$$

where the time-independent \( H_0 \) contains kinetic energy, scalar potential and SOI. The time-dependence of the Hamiltonian arises from the precession of magnetization, which points in direction \( \dot{r}(t) \). \( m = -\mu_B \sigma \) with the Bohr magneton \( \mu_B \) and the vector of Pauli spin matrices \( \sigma = (\sigma_x, \sigma_y, \sigma_z)^T \) is the magnetic moment operator. \( \Omega^{xc}(r) \) is the exchange field, i.e., the difference between the potentials of majority and minority electrons \( \Omega^{xc}(r) = \frac{1}{2m} \left( V_{\text{minority}}(r) - V_{\text{majority}}(r) \right) \). Around the time \( t_0 \) we can approximate the motion of \( \dot{r}(t) \) by

$$\dot{r}(t) \approx \frac{d \dot{r}(t)}{dt} \bigg|_{t=t_0} \approx \frac{d \dot{r}(t)}{dt} \bigg|_{t=t_0} \sin(\omega \Delta t) \omega,$$

for small time changes \( \Delta t \) and with a small arbitrary frequency \( \omega \Delta t \ll 1 \). Likewise, the Hamiltonian can be approximated as

$$H(r, t) \approx H(r, t_0) - m \cdot \dot{r}(t_0) \Omega^{xc}(r) \approx \frac{d \dot{r}(t)}{dt} \bigg|_{t=t_0} \Omega^{xc}(r) \sin(\omega \Delta t) \omega.$$

The \( \Delta t \)-dependent term

$$V(r, \Delta t) = -m \cdot \frac{d \dot{r}(t)}{dt} \bigg|_{t=t_0} \Omega^{xc}(r) \sin(\omega \Delta t) \omega$$

$$= -m \cdot \dot{r}(t_0) \times \frac{d \dot{r}(t)}{dt} \bigg|_{t=t_0} \Omega^{xc}(r) \sin(\omega \Delta t) \omega$$

$$= \frac{\sin(\omega \Delta t)}{\omega} \left( \dot{r}(t_0) \times \frac{d \dot{r}(t)}{dt} \bigg|_{t=t_0} \right) \cdot \dot{r}(t)$$

acts as a time-dependent perturbation on the eigenstates of \( H(r, t_0) \). Here, \( \dot{T}(r) = \dot{r} \times \dot{M}(t_0) \Omega^{xc}(r) \) is the torque operator.

Within linear response the current density in \( \sigma \) direction, \( j_\sigma \), induced by the time-dependent perturbation Eq. (4) is given by

$$j_\sigma(t_0) = e \lim_{\omega \to 0} \left. \frac{\text{Im} G^{R}_{\sigma, \omega, \dot{r} \cdot \dot{M}}(\omega, \dot{M}(t_0))}{\hbar \omega} \right|_{\dot{M}(t_0)} \left( \dot{M}(t_0) \times \frac{d \dot{M}}{dt} \bigg|_{t=t_0} \right) \beta \beta,$$

where \( e > 0 \) is the elementary positive charge, \( V \) is the volume and \( G^{R}_{\sigma, \omega, \dot{r} \cdot \dot{M}}(\omega, \dot{M}) \) is the Fourier transform of the retarded velocity-torque correlation function, i.e.,

$$G^{R}_{\sigma, \omega, \dot{r} \cdot \dot{M}}(\omega, \dot{M}) = -i \int_0^\infty dt e^{i \omega t} \langle [v_\sigma(t), \dot{T}_\beta(0)] \rangle,$$

evaluated for the time-independent Hamiltonian

$$H_M(r) = H_0(r) - m \cdot \dot{M} \Omega^{xc}(r)$$

in terms of the Fourier transform of the retarded torque-velocity correlation function

$$G^{R}_{\sigma, \omega, \dot{r} \cdot \dot{M}}(\omega, \dot{M}) = -i \int_0^\infty dt e^{i \omega t} \langle [\dot{T}_\sigma(t), v_\beta(0)] \rangle$$

of a system with magnetization in direction \( \dot{M} \).

Next, we compare Eq. (5) to the expressions describing SOTs. Within linear response to an applied electric field \( E \) the SOT on the magnetization is \( T(\dot{M}) = t(\dot{M})E \), where the torque tensor \( t(\dot{M}) \) is given by

$$t_{\alpha \beta}(\dot{M}) = e \left. \frac{\text{Im} G^{R}_{\sigma, \omega, \dot{r} \cdot \dot{M}}(\omega, \dot{M})}{\hbar \omega} \right|_{\dot{M}(t_0)} \langle v_\sigma(t), T_\beta(0) \rangle.$$
This identity allows us to rewrite the magnetization-dynamics induced current density, Eq. (5), in terms of the torkance tensor as

\[
\dot{j}_a(t) = \frac{1}{V} \sum_\beta t_{j_a}(-\dot{\mathbf{M}}(t)) \left( \dot{\mathbf{M}}(t) \times \frac{d\dot{\mathbf{M}}(t)}{dt} \right)_\beta.
\]

(14)

It is thus very convenient to discuss both SOT and ISOT in terms of the torkance tensor. We note in passing that the torque-velocity correlations, which the torkance measures, govern also the Dzyaloshinskii-Moriya interaction.\textsuperscript{36,37}

In the discussion of bilayer systems below we will consider in addition to \(j_a\) the current per length \(I_a/\ell\), which is obtained by replacing the current density operator \(-ev_\alpha/V\) by \(-ev_\alpha/A\):

\[
\frac{I_a(t)}{\ell} = \frac{1}{A} \sum_\beta t_{j_a}(-\dot{\mathbf{M}}(t)) \left( \dot{\mathbf{M}}(t) \times \frac{d\dot{\mathbf{M}}(t)}{dt} \right)_\beta,
\]

(15)

where \(A\) is the cross sectional area of the unit cell of the bilayer normal to the stacking direction. Since the atom-resolved current is expected to vary significantly between atomic layers in bilayer systems, \(I_a/\ell\) is a suitable definition of current density in such systems. It is convenient to decompose the torkance tensor into two components that are even and odd with respect to magnetization reversal, respectively \(I_a^{\text{even}}(t)\) and \(I_a^{\text{odd}}(t)\), where \(I_a^{\text{even}}(\mathbf{M}) = [t(\mathbf{M}) + t(-\mathbf{M})]/2\) and \(I_a^{\text{odd}}(\mathbf{M}) = [t(\mathbf{M}) - t(-\mathbf{M})]/2\). Separating \(I_a/\ell\) into the components due to \(I_a^{\text{even}}(\mathbf{M})\) and \(I_a^{\text{odd}}(\mathbf{M})\) yields

\[
\frac{I_a^{\text{even}}(t)}{\ell} = \frac{1}{A} \sum_\beta t_{j_a}^{\text{even}}(\dot{\mathbf{M}}(t)) \left( \dot{\mathbf{M}}(t) \times \frac{d\dot{\mathbf{M}}(t)}{dt} \right)_\beta,
\]

\[
\frac{I_a^{\text{odd}}(t)}{\ell} = -\frac{1}{A} \sum_\beta t_{j_a}^{\text{odd}}(\dot{\mathbf{M}}(t)) \left( \dot{\mathbf{M}}(t) \times \frac{d\dot{\mathbf{M}}(t)}{dt} \right)_\beta.
\]

(16)

III. SOT AND ISOT IN BILAYER SYSTEMS

In the following we discuss SOT and ISOT in magnetic bilayer systems composed of a ferromagnetic layer (FM) deposited on a normal metal (NM). When the electric field \(\mathbf{E} = E_\parallel \mathbf{e}_x\) is applied in-plane along \(x\) direction, the torques satisfy

\[
\mathbf{T}^{\text{even}}(\mathbf{M}) = E_\parallel \dot{\mathbf{M}} \times (\mathbf{e}_x \times \mathbf{M}) \left[ A_0 + A_2 (\mathbf{e}_x \times \mathbf{M})^2 + \cdots \right] +
\]

\[
+ E_\parallel (\dot{\mathbf{M}} \times \mathbf{e}_x) \left( \dot{\mathbf{M}} \times \mathbf{e}_x \right) \left[ B_2 + B_4 (\mathbf{e}_x \times \mathbf{M})^2 + \cdots \right]
\]

(17)

and

\[
\mathbf{T}^{\text{odd}}(\mathbf{M}) = E_\parallel (\dot{\mathbf{M}} \times \mathbf{e}_x) \left[ C_0 + C_2 (\mathbf{e}_x \times \mathbf{M})^2 + \cdots \right] +
\]

\[
+ E_\parallel \dot{\mathbf{M}} \times (\mathbf{e}_x \times \mathbf{M}) \left[ D_2 + D_4 (\mathbf{e}_x \times \mathbf{M})^2 + \cdots \right]
\]

(18)

in bilayer systems composed of polycrystalline, disordered or amorphous layers with continuous rotational symmetry around the \(z\) axis.\textsuperscript{35}

In the following we discuss the magnetization-dynamics induced current density \(I_a/\ell\) in \(x\) direction. Using Eq. (17) and Eq. (13) in Eq. (16) we obtain

\[
\frac{I_a^{\text{even}}(t)}{\ell} = \frac{A_0}{A} \left[ \mathbf{M} \times (\mathbf{e}_y \times \mathbf{M}) \right] \cdot \left[ \dot{\mathbf{M}} \times \frac{d\dot{\mathbf{M}}}{dt} \right] +
\]

\[
+ \frac{A_2}{A} \left[ \mathbf{M} \times (\mathbf{e}_y \times \mathbf{M}) \right] \cdot \left[ \dot{\mathbf{M}} \times \frac{d\dot{\mathbf{M}}}{dt} \right] (\mathbf{e}_x \times \mathbf{M})^2 +
\]

\[
+ \frac{B_2}{A} (\dot{\mathbf{M}} \times \mathbf{e}_x) \cdot \left[ \dot{\mathbf{M}} \times \frac{d\dot{\mathbf{M}}}{dt} \right] (\mathbf{M} \times \mathbf{e}_x) +
\]

\[
+ \frac{B_4}{A} (\dot{\mathbf{M}} \times \mathbf{e}_x) \cdot \left[ \dot{\mathbf{M}} \times \frac{d\dot{\mathbf{M}}}{dt} \right] (\mathbf{M} \times \mathbf{e}_x)^2 + \cdots
\]

(19)

and

\[
\frac{I_a^{\text{odd}}(t)}{\ell} = -\frac{C_0}{A} (\mathbf{e}_y \times \mathbf{M}) \cdot \left[ \dot{\mathbf{M}} \times \frac{d\dot{\mathbf{M}}}{dt} \right] (\mathbf{e}_x \times \mathbf{M})^2 +
\]

\[
- \frac{C_2}{A} (\mathbf{e}_y \times \mathbf{M}) \cdot \left[ \dot{\mathbf{M}} \times \frac{d\dot{\mathbf{M}}}{dt} \right] (\mathbf{M} \times \mathbf{e}_x) +
\]

\[
- \frac{D_2}{A} \left[ \mathbf{M} \times (\mathbf{M} \times \mathbf{e}_x) \right] \cdot \left[ \dot{\mathbf{M}} \times \frac{d\dot{\mathbf{M}}}{dt} \right] (\mathbf{M} \times \mathbf{e}_x)^2 + \cdots.
\]

(20)

A. Current densities induced by FMR through the inverse SOT

First, we consider the case of FMR-driven magnetization precession around the \(z\) axis in a circular orbit, i.e.,

\[
\mathbf{M}(t) = [\sin(\theta) \cos(\omega t), \sin(\theta) \sin(\omega t), \cos(\theta)]^T,
\]

(21)

where \(\theta\) is the cone angle. Inserting Eq. (21) into Eqs. (19) and (20) we obtain

\[
\frac{I_a^{\text{even}}(t)}{\ell} = -\frac{\omega}{A} \sin(\theta) \cos(\omega t) \sin(\omega t) \{ A_0 + A_2 \sin^2(\theta) + \cdots \},
\]

\[
\frac{I_a^{\text{odd}}(t)}{\ell} = \frac{\omega}{A} \sin(\theta) \cos(\omega t) \{ C_0 + C_2 \sin^2(\theta) + \cdots \} +
\]

\[
+ \frac{\omega}{A} \sin(\theta) \cos(\omega t) \{ D_2 \sin^2(\theta) + D_4 \sin^4(\theta) + \cdots \}.
\]

(22)

For small cone angles \(\theta\) the \(\sin^2(\theta)\) factors suppress the contributions from \(A_2, C_2, D_2\) and further higher-order terms. In the small cone limit the ISOT for magnetization precession around the \(z\) axis can thus be expressed in terms of the torkance for magnetization along \(z\), if \(A_0 = t^{\text{even}}(\mathbf{M} = \mathbf{e}_z)\) and \(C_0 = t^{\text{odd}}(\mathbf{M} = \mathbf{e}_z)\) are used. Experiments\textsuperscript{15,16} and \textit{ab initio} calculations\textsuperscript{22} have found that \(A_0\) and \(C_0\) can be of the same order of magnitude in AlO\(_x\)/Co/Pt and MgO/CoFeB/Ta. The two contributions \(I_a^{\text{even}}(t)/\ell\) and \(I_a^{\text{odd}}(t)/\ell\) are therefore expected to exhibit similar amplitudes. Since \(I_a^{\text{even}}(t)/\ell \propto \)
sin(ωt) while \( I_{\text{even}}^\text{odd}(t)/\ell \propto \cos(\omega t) \) the even and odd part are phase-shifted with respect to each other.

Next, we consider FMR-driven magnetization precession around the y axis. In this case the magnetization follows an elliptical trajectory in thin bilayer films due to the demagnetization field,\(^{36}\)

\[
\mathbf{M}(t) = [\sin(\theta) \sin(\omega t)\epsilon, \cos(\theta), \sin(\theta) \cos(\omega t)]^T, \tag{23}
\]

where \( \epsilon \) is the ratio of the major axis to the minor axis of the ellipse. The resulting induced current density is given by

\[
I_{\text{even}}^\text{odd}(t)/\ell = \frac{\omega}{A} \sin^2(\theta)\epsilon \left[ 1 - \sin^2(\theta) \sin^2(\omega t)(1 - \epsilon^2) \right]\left[ A_0 + A_1 \cos^2(\theta) + A_2 \sin^2(\theta) \sin^2(\omega t) \right] + \cdots
- \frac{\omega}{2A} \sin^2(\theta)\epsilon \left[ 1 + \sin^2(\theta)(\epsilon^2 - 1) \right]\left[ B_2 + B_4 \cos^2(\theta) + B_4 \sin^2(\theta) \sin^2(\omega t) \right] + \cdots, \tag{24}
\]

\[
I_{\text{odd}}(t)/\ell = \frac{\omega}{2A} \sin^2(\theta)\epsilon \left[ 1 - \sin^2(\theta) \sin^2(\omega t) \right]\left[ C_0 + C_2 \cos^2(\theta) + C_4 \sin^2(\theta) \sin^2(\omega t) \right] + \cdots
- \frac{\omega}{2A} \sin^2(\theta)\epsilon \left[ 1 + \sin^2(\theta)(\epsilon^2 - 1) \right]\left[ D_2 + D_4 \cos^2(\theta) + D_4 \sin^2(\theta) \sin^2(\omega t) \right] + \cdots. \tag{25}
\]

For small angles \( \theta \) the terms proportional to \( \sin^2(\theta) \) dominate while terms proportional to \( \sin^2(\theta) \) and higher are suppressed. Thus we can approximate in the small-cone limit

\[
I_{\text{even}}^\text{odd}(t)/\ell = \frac{\omega}{A} \sin^2(\theta)\epsilon [A_0 + A_2 + A_4 + \cdots]
- \frac{\omega}{2A} \sin^2(\theta)\epsilon [B_2 + B_4 + \cdots].
\]

\[
I_{\text{odd}}(t)/\ell = \frac{\omega}{2A} \sin^2(\theta)\epsilon [C_0 + C_2 + \cdots]
- \frac{\omega}{2A} \sin^2(\theta)\epsilon [D_2 + D_4 + \cdots].
\]

\( I_{\text{even}}^\text{odd}/\ell \) is the sum of a dc component and an ac component with frequency \( 2\omega \), while \( I_{\text{odd}}^\text{odd}/\ell \) consists of only an ac part with frequency \( 2\omega \). The ac components of the even and odd part are phase shifted. Compared to the induced current for precession around the \( z \) axis, Eq. (23a), the amplitude is expected to be typically reduced by roughly a factor of \( \sin(\theta) \) when the magnetization precesses around the \( y \) axis. The dc component of the voltage \( -R_{xy}I_{\text{even}} \), where \( R_{xy} \) is the resistance, has been measured for several bilayer systems and is usually interpreted as the voltage arising from the conversion of pumped dc spin current via the ISHE.\(^{26,27}\)

We turn now to the FMR-driven magnetization precession around the \( x \) axis. Again, the magnetization follows an elliptical trajectory,

\[
\mathbf{M}(t) = [\cos(\theta), \sin(\theta) \cos(\omega t)\epsilon, \sin(\theta) \sin(\omega t)]^T, \tag{26}
\]

with \( \epsilon \) the ratio of major axis to minor axis of the ellipse. In this case the current density induced by the precessing magnetization is given by

\[
I_{\text{even}}(t)/\ell = -\frac{\omega}{2A} \epsilon \sin(\theta)\sin(\theta) \left[ 1 - \sin^2(\theta)(1 - \epsilon^2) \cos^2(\omega t) \right] \times \left[ A_0 + A_2 \cos^2(\theta) + A_4 \sin^2(\theta) \sin^2(\omega t) \right] + \cdots
+ \frac{\omega}{2A} \epsilon \sin(\theta)\sin(\theta) \left[ 1 + \sin^2(\theta)(\epsilon^2 - 1) \right] \times \left[ B_2 + B_4 \cos^2(\theta) + B_4 \sin^2(\theta) \sin^2(\omega t) \right] + \cdots. \tag{27}
\]

In the small-cone limit we obtain

\[
I_{\text{even}}(t)/\ell = -\frac{\omega}{2A} \epsilon \sin(\theta)\sin(\theta) \left[ C_0 + C_2 \cos^2(\theta) + C_4 \sin^2(\theta) \sin^2(\omega t) \right] + \cdots
- \frac{\omega}{A} \epsilon \sin(\theta)\sin(\theta) \left[ 1 + \sin^2(\theta)(\epsilon^2 - 1) \right] \times \left[ D_2 + D_4 \cos^2(\theta) + D_4 \sin^2(\theta) \sin^2(\omega t) \right] + \cdots. \tag{28}
\]

Even if \( A_2, B_2, C_2 \) and \( D_2 \) are non-zero, i.e., even in the presence of anisotropic SOT, the ISOT for magnetization precession around the \( x \) axis can thus be expressed in terms of the torkance for magnetization along \( x \). The even and odd contributions are again phase-shifted and the dependence on the cone angle is \( \propto \sin(\theta) \) in the limit of small \( \theta \) like in the case of magnetization precession around the \( z \) axis, promising a significantly larger ISOT signal\(^{26}\) compared to the case with magnetization precession around the \( y \) axis.

In all cases considered above, the coefficients \( C_0, C_2, \ldots \) and \( D_2, D_4, \ldots \), which govern the odd torkance, give rise to an ac current, but never to a dc current. Thus, complete characterization of ISOT in experiments requires the measurement of the ac component.

B. Consequences of the reciprocity between SOT and ISOT for the spatial spin current density decay and the SHE angles

In magnetic bilayer systems that involve a normal metal layer with large SHE it is expected that an important contribution to SOT arises from SHE. Conversely, the combined action of spin pumping and ISHE contributes to ISOT. In the following we use the reciprocity between SOT and ISOT to establish a connection between phenomenological models that have been developed to describe the SHE/ISHE-related contributions to SOT on the one hand and to ISOT on the other hand.
We consider a bilayer system composed of a ferromagnetic layer (FM) on a semi-infinite normal metal (NM). The interface between FM and NM is located at \( z = 0 \). First, we estimate the SOT arising from the SHE generated by an applied electric field \( E_x \), \( \hat{e}_x \), in \( x \) direction. Deep inside NM, i.e., for \( z \ll 0 \), the spin current density flowing in \( z \) direction is

\[
Q_z = \sigma^{xy}_x E_x = \frac{\hbar}{2e} \sigma^{xx}_x E_x \tan \gamma_{\text{SHE}}
\]

where \( \sigma^{xy}_x \) is the SHE conductivity in NM, \( \gamma_{\text{SHE}} \) is the SHE angle and \( \sigma^{xx}_x \) is the normal conductivity in NM. We assume that a fraction \( \xi \) of \( Q_z \) is absorbed by FM, thereby causing a torque on its magnetization, which we assume to point in \( z \) direction. \( \xi \) can be thought of as the SHE-to-SOT conversion efficiency. Denoting the \( xy \) cross sectional area of the unit cell by \( A \), the torque per unit cell is given by \( T_y = \xi A Q_z = t_y E_x \) with

\[
t_y = \xi \sigma^{xy}_x = \frac{\hbar}{2e} \sigma^{xx}_x \tan \gamma_{\text{SHE}}.
\]

Next, we consider the ISOT arising from the combined action of spin pumping and ISHE. The spin current density pumped adiabatically into NM is determined by

\[
Q(z = 0) = \frac{\hbar}{4\pi} \text{Re} g^{\dagger} \mathbf{M} \times \frac{d\mathbf{M}}{dt}.
\]

where \( g^{\dagger} \) is the (generally complex) spin mixing conductance per cross sectional area. The imaginary part of \( \gamma_{\text{SHE}} \) is negligible in Eq. (31). If spin transport in NM is di

g
dependent of \( z \), the spin current density pumped into NM is determined by

\[
Q_y = -\frac{\hbar \omega}{4\pi} \text{Re} g^{\dagger} \sin^2(\theta) e^{i\lambda_{sd}}.
\]

Due to ISHE this spin current is converted into an in-plane charge current flowing in \( x \) direction:

\[
j_x(z) = -\frac{2e}{\hbar} Q_y(z) \tan \gamma_{\text{ISHE}} = \frac{e\omega}{2\pi} \text{Re} g^{\dagger} \sin^2(\theta) e^{i\lambda_{sd}} \tan \gamma_{\text{ISHE}}
\]

where \( \gamma_{\text{ISHE}} \) is the ISHE-angle. Thus, a single characteristic length, the spin diffusion length \( \lambda_{sd} \), determines the position dependence of \( s(z) \), \( Q_y(z) \) and \( j_x(z) \) within this model:

\[
j_x(z) \propto Q_y(z) \propto s(z) \propto e^{j\lambda_{sd}}.
\]

Integration of the current density Eq. (33) from \( z = -\infty \) to \( z = 0 \) yields the current per length flowing in NM:

\[
\frac{I_x}{\ell} = \frac{e\omega}{2\pi} \text{Re} g^{\dagger} \sin^2(\theta) \lambda_{sd} \tan \gamma_{\text{ISHE}}.
\]

Using the small-cone limit of Eq. (24) and assuming \( A_2 = B_2 = A_4 = \cdots = 0 \) we obtain the alternative expression

\[
\frac{I_x}{\ell} = \frac{\omega}{A} \sin^2(\theta) eA_0.
\]

Equating the two expressions for \( I_x / \ell \) yields

\[
A_0 = \frac{A}{2\pi} \text{Re} g^{\dagger} \lambda_{sd} \tan \gamma_{\text{ISHE}}.
\]

Using \( t_y(\mathbf{M} = \hat{e}_x) = A_0 \) leads to

\[
\lambda_{sd} = \frac{2\pi t_y(\mathbf{M} = \hat{e}_x)}{eA \text{Re} g^{\dagger} \tan \gamma_{\text{ISHE}}}
\]

Remarkably, our model Eq. (30) for the SHE contribution to SOT is conceptually independent of \( \lambda_{sd} \): The fraction \( \xi \) of spin current from the SHE in NM is converted into a torque on the magnetization in FM. This SHE spin current in NM is independent of \( z \) for \( z \ll 0 \) and only determined by the applied in-plane electric field and the SHE conductivity. Without invoking a finite value of \( \lambda_{sd} \) one can thus conclude that a ferromagnetic layer deposited on the semi-infinite NM layer is subject to a well-defined SOT contribution due to SHE, which enters via \( t_y(\mathbf{M} = \hat{e}_x) \) into Eq. (33). Conversely, for given non-zero spin mixing conductance and \( \gamma_{\text{SHE}} \) the ISOT current induced by magnetization dynamics is limited by \( \lambda_{sd} \). An infinite value of \( \lambda_{sd} \) would lead to infinite ISOT current. Reciprocity between the SHE/ISHE-mediated contributions to SOT and ISOT fixes the value of \( \lambda_{sd} \) according to Eq. (39).

Using Eq. (30) and assuming \( \gamma_{\text{ISHE}} = \gamma_{\text{SHE}} \) we can recast Eq. (39) as

\[
\lambda_{sd} = \frac{\xi \hbar n \sigma^{xx}_x}{e^2 \text{Re} g^{\dagger}}.
\]

Solely on the grounds of reciprocity between SOT and ISOT this expression relates \( \lambda_{sd} \) and \( \sigma^{xx}_x \). In Eq. (29) the conductivity \( \sigma^{xx}_x \) limits the spin current from which the torque arises and in Eq. (33) \( \lambda_{sd} \) limits the region of space in which the spin current is converted into a charge current, thereby limiting the total charge current produced by ISHE. Reciprocity between SOT and ISOT then dictates that these two limiting factors be related, \( \lambda_{sd} \propto \sigma^{xx}_x \), with the factor of proportionality given in terms of the efficiency \( \xi \) of SOT generation by SHE currents on the one hand and the spin pumping efficiency \( \text{Re} g^{\dagger} \) on the other hand. Since the existence of SHE/ISHE is the only vital assumption in the derivation, Eq. (39) states that SHE/ISHE will lead to an finite spin diffusion length in systems with finite conductivity \( \sigma^{xx}_x \) irrespective of the scattering mechanism limiting \( \sigma^{xx}_x \). In other words, Eq. (39) captures spin relaxation through ISHE.

Several additional spin relaxation mechanisms\(^{29,40}\) by various spin-flip processes not captured by Eq. (39) suppress \( \lambda_{sd} \) further. In order to include them into Eq. (39) we observe that the SHE angle in Eq. (29) has to describe the charge-to-spin-current conversion in the presence of all spin relaxation mechanisms: The spin current flowing in NM is determined by the interplay of spin current generation by SHE on
the one hand and spin current annihilation by spin relaxation on the other hand. In contrast, \( \lambda_{sd} \) in Eq. (35) captures all spin relaxation mechanisms and thus we have to take care not to double-count the effect of spin current annihilation when specifying the ISHE angle in Eq. (33). For this purpose we define \( \gamma_{SHE} \), which describes charge-to-spin-current conversion without taking spin current annihilation into account. The generalization of Eq. (39) is then given by

\[
\lambda_{ad} = \frac{\varepsilon_0 n\sigma_{xx}}{\varepsilon e^2 R_{\text{ISHE}}} \tan \gamma_{SHE},
\]

where \( \tan \gamma_{SHE} \approx \tan \gamma_{ISHE} \leq 1 \).

In order to formalize the relation between \( \gamma_{SHE} \) and \( \gamma_{ISHE} \) we employ the Kubo formalism used in Sec. II. We consider a normal metal NM and assume that spin transport is diffusive in NM. The presence of a spin current \( Q_z \) flowing in \( z \) direction is associated with a gradient of the spin quasichemical potential

\[
\frac{1}{\hbar} \frac{\partial}{\partial z} \left[ \mu_\parallel(z) - \mu_\perp(z) \right] = - \frac{2 e^2 Q_y}{\hbar \sigma_{zz}},
\]

where \( \mu_\parallel(z) \) is the quasichemical potential of spins pointing in \( y \) direction and \( \mu_\perp(z) \) the one of spins pointing in \( -y \) direction. The gradients of the quasichemical potential act like a spin-dependent effective electric field in \( z \) direction

\[
E_z = \frac{1}{\hbar} \frac{\partial \mu_\parallel(z)}{\partial z} = - \frac{2 e Q_y}{\hbar \sigma_{zz}},
\]

where \( s = +1 \) for spin in \( y \) direction and \( s = -1 \) for spin in \( -y \) direction. Within linear response the charge current density in \( x \) direction induced by this effective electric field is given by

\[
j_x = \frac{e^3}{h} \lim_{\omega \to 0} \frac{\text{Im} G^R_{\nu_\parallel \nu_\perp} (\omega)}{\sigma_{zz}}.
\]

where \( \{\nu_\parallel, \nu_\perp\} = \nu_\parallel \sigma_y + \sigma_y \nu_\parallel \) is the anticommutator of \( \nu_\parallel \) and \( \sigma_y \). The corresponding ISHE angle is determined by

\[
\tan \gamma_{ISHE} = - \hbar \lim_{\omega \to 0} \frac{2 e j_x}{2 Q_y} \frac{\text{Im} G^R_{\nu_\parallel \nu_\parallel \nu_\perp \nu_\perp} (\omega)}{\hbar \omega}.
\]

The SHE conductivity is given by

\[
\sigma_{zz} = e \lim_{\omega \to 0} \frac{\text{Im} G^R_{\nu_\parallel \nu_\perp} (\omega)}{\hbar \omega},
\]

where \( Q_y \) is the spin current density operator for spin current flowing in \( z \) direction with spin pointing in \( y \) direction. If \( \sigma_y \) approximately commutes with the Hamiltonian we can use

\[
Q_y = \frac{\hbar}{4V} \{\nu_\parallel, \sigma_y\}
\]

and obtain (provided \( \sigma_{xx} = \sigma_{zz} \) holds)

\[
\tan \gamma_{SHE} = \frac{\text{Im} G^R_{\nu_\parallel \nu_\perp \nu_\parallel \nu_\perp} (\omega)}{\hbar \omega}.
\]

In the presence of strong spin-flip scattering Eq. (46) overestimates the spin current. One can even construct examples where Eq. (46) yields a non-zero spin current in the absence of any spin transport. Thus, \( \tan \gamma_{SHE} \leq \tan \gamma_{ISHE} \) in general.

C. Joule heating from ISOT

We consider a bilayer composed of a thin ferromagnet (FM) on a normal metal (NM) of thickness \( D \). Magnetization is assumed to precess around the \( z \) axis according to Eq. (21). The microwave excitation power per area is

\[
P_{\text{FMR}} = \frac{\hbar}{4\pi} R_{\text{ISHE}} \sin^2(\theta) \omega^2,
\]

assuming that spin pumping is the only damping mechanism present. In NM the spin currents

\[
Q_x(z) = \frac{\hbar}{4\pi} R_{\text{ISHE}} \sin^2(\theta) \cos(\theta) \omega \sin(\omega t) e^{i \omega t},
\]

flow in \( z \) direction, where the boundary between FM and NM is again located at \( z = 0 \). ISHE converts \( Q_x(z) \) into a charge current density flowing in \( y \) direction and \( Q_y(z) \) into one flowing in \( x \) direction. The resulting total in-plane current is rotating around the \( z \) axis due to the phase difference between \( Q_x(z) \) and \( Q_y(z) \). The amplitude of this rotating charge current density is given by

\[
j(z) = \frac{e}{2\pi} R_{\text{ISHE}} \sin^2(\theta) \cos(\theta) \omega e^{i \omega t} \tan \gamma_{ISHE}.
\]

The total current per length flowing in-plane is the integral of \( j(z) \) from \(-D\) to \( D\) and amounts to

\[
\frac{I}{\ell} = \frac{e}{2\pi} R_{\text{ISHE}} \sin^2(\theta) \cos(\theta) \omega \left[ 1 - e^{-D/\lambda_{sd}} \right] \lambda_{sd} \tan \gamma_{ISHE}.
\]

This electric current \( I \) induced by the FMR-driven ISOT leads to Joule heating \( P_{\text{el}} = R^2I^2 \), where \( R \) is the resistance of the bilayer. Conservation of energy requires \( P_{\text{el}} \leq P_{\text{FMR}} \). Assuming that the resistivity of FM is much larger than the resistivity \( \rho \) of NM, we obtain in the small-cone limit

\[
P_{\text{FMR}} = \frac{e^2}{\pi \hbar} R_{\text{ISHE}} \lambda_{sd} \rho \left[ \tan \gamma_{ISHE} \right]^2 \hbar \left( \frac{D}{\lambda_{sd}} \right),
\]

where the function

\[
h(\xi) = \frac{1 - e^{-\xi^2}}{\xi}
\]

has a maximum of 0.41.

Above, we neglected the backscattering of spin current, assuming that the spin current simply disappears as it reaches the bottom of NM at \( z = -D \). This artificial disappearance of spin current at the bottom of NM is associated with a disappearance of power. In order to account correctly for all the power we assume now that NM is infinitesimally thin and that below NM a perfect spin sink is located. The power carried by the spin current is proportional to the square of its amplitude. Thus, the power lost while traversing NM is

\[
\delta P_{\text{FMR}} = 2DP_{\text{FMR}}/\lambda_{sd}.
\]

Assuming that FM and the perfect
spin sink have infinite resistivity, the ratio of Joule heating in NM, \( \delta P_{el} \), to \( \delta P_{FMR} \) is given by

\[
\frac{\delta P_{el}}{\delta P_{FMR}} = \frac{e^2}{2\pi\hbar} \text{Reg}^{14} \lambda_{ad} \left[ \tan \gamma_{\text{ISHE}} \right]^2 ,
\]

which is slightly larger than the maximum of Eq. (52). Using Eq. (54) leads to the condition

\[
\frac{\delta P_{el}}{\delta P_{FMR}} = \frac{\xi}{2} \tan \gamma_{\text{ISHE}} \tan \gamma_{\text{SHE}} \leq 1 .
\]

SHE-angles observed so far experimentally in metallic systems are below the limit set by Eq. (55). Even for a comparatively large SHE of \( \tan \gamma_{\text{ISHE}} = \tan \gamma_{\text{SHE}} = 0.2 \), the Joule heating accompanying the ISHE voltage contributes only of the order of one percent to the dissipation of the microwave excitation power.

The Joule heating is proportional to \( \lambda_{ad} \) according to Eq. (54) because \( \lambda_{ad} \) determines the size of the region in which \( P_{el} \) arises. An infinite value of \( \lambda_{ad} \) would therefore allow us to harvest more Joule heat than the invested microwave excitation energy, which is impossible. Therefore the presence of ISHE limits \( \lambda_{ad} \) for reasons of energy conservation. Earlier, in the discussion of Eq. (59), we pointed out that \( \lambda_{ad} \) has to be finite such that not more and not less current is produced by ISOT than dictated by reciprocity with SOT. In this sense, the constraints imposed on \( \lambda_{ad} \) by energy conservation and reciprocity in the presence of ISHE, are similar in character. However, the constraint arising from energy conservation becomes active only when the SHE angles reach the order of 1.

IV. FIRST PRINCIPLES CALCULATIONS

A. Computational details

In the following we will discuss SOTs and ISOTs for a bilayer composed of 3 layers of hcp Co on 20 layers of fcc Pt(111), denoted in the following as Co(3)/Pt(20). Sputter deposited Pt typically shows a strong (111) texture along the growth direction, which motivates our choice of the (111) orientation for the fcc Pt layer, which is 4.5 nm thick in our calculation. We determined the electronic structure self-consistently within the generalized gradient approximation to density functional theory using the full-potential linearized augmented-plane-wave program FLEUR. The film mode of FLEUR, which treats the vacuum regions explicitly, was employed. Muffin tin (MT) radii of 2.6 \( a_0 \) for Pt and 2.18 \( a_0 \) for Co were used in the calculation and the plane-wave cutoff was set to 3.8 \( a_0^{-1} \), where \( a_0 \) is Bohr’s radius. The Brillouin zone was sampled by a 24\texttimes24 Monkhorst-Pack \( k \)-mesh and spin-orbit interaction was treated within second variation. The experimental in-plane lattice constant of Pt(111) of 5.24 \( a_0 \) was used. The interlayer distance in Pt(111) was set to the experimental value of 4.28 \( a_0 \). For the Co layer we assumed hcp stacking and that the first two atomic layers of Co follow the fcc pattern of Pt(111), i.e., the Co layer is stacked like ABA onto the Pt layer with termination ABC. The Co/Pt interface was relaxed in the out-of-plane direction yielding a distance of 3.89 \( a_0 \) between the Pt and Co interface layers. We label the atomic planes of the Pt layer by Pt1 through Pt20, where Pt20 is at the Co/Pt interface. Likewise, we label the atomic planes of the Co layer by Co1 through Co3, where Co1 is at the Co/Pt interface. We introduce a cartesian coordinate system such that the \( z \) axis is perpendicular to the atomic planes, i.e., along the out-of-plane direction. Additionally, Pt1 has a smaller \( z \) coordinate than Co3, i.e., the Pt layer is below the Co layer. The magnetization direction is set to \( \hat{M} = \hat{e}_z \) in the calculation. We find the magnetic moments in units of \( \mu_B \) (Bohr magneton) to be 0.03 (Pt18), 0.10 (Pt19), 0.25 (Pt20), 1.86 (Co1), 1.84 (Co2) and 1.90 (Co3).

Within the independent particle approximation the torque \( t \) defined in Eq. (8) can be expressed as sum of three terms, \( t_{\alpha\beta} = t_{\alpha\beta}^{(a)} + t_{\alpha\beta}^{(b)} + t_{\alpha\beta}^{(M)} \), where

\[
t_{\alpha\beta}^{(a)} = \frac{e}{N\hbar} \sum_k \text{Tr} \left\{ T_{\alpha k} G^R_k(E_F) v_{\beta k} G^A_k(E_F) \right\},
\]

\[
t_{\alpha\beta}^{(b)} = \frac{e}{N\hbar} \sum_k \text{Re} \text{Tr} \left\{ T_{\alpha k} G^R_k(E_F) v_{\beta k} G^A_k(E_F) \right\},
\]

\[
t_{\alpha\beta}^{(M)} = \frac{e}{N\hbar} \sum_k \int_{-\infty}^{E_F} dE \text{Re} \text{Tr} \left\{ T_{\alpha k} G^R_k(E) v_{\beta k} \frac{dG^R_k(E)}{dE} \right\} - \mathcal{T}_{\alpha\beta} \frac{dG^A_k(E)}{dE} v_{\beta k} G^R_k(E),
\]

with \( G^R_k(E) \) the retarded Green function at \( k \) point \( k \) and energy \( E \), \( G^A_k(E) \) the advanced one, \( N \) the number of \( k \) points and \( E_F \) the Fermi energy. Recent first principles calculations based on Eq. (56) for the SOT in Co/Pt(111) systems are in satisfactory agreement with experiments.

In order to evaluate Eq. (56) computationally efficiently, the Wannier interpolation technique is employed. Per atom 18 maximally localized Wannier functions (MLWFs) were constructed from an 8\times8 \( k \)-point mesh by disentanglement from 800 bands. We model the effect of disorder by a phenomenological band broadening \( \Gamma \) in the Green functions, i.e., \( G^R_k(E) = \frac{1}{\hbar} \left[ E - H_k + \mathcal{I} \right]^{-1} \). Within the Wannier interpolation scheme, Hamiltonian \( H_k \), velocity operator \( v_{\alpha\beta} \) and torque operator \( \mathcal{T}_{\alpha\beta} \) are obtained from

\[
H_{\text{Wann}} = \sum_{R} e^{R} \langle W_{\text{mo}}|H|W_{\text{mR}} \rangle,
\]

\[
v_{\text{Wann}} = \frac{1}{N} \sum_{R} e^{R} iR_{\alpha} \langle W_{\text{mo}}|H|W_{\text{mR}} \rangle,
\]

\[
\mathcal{T}_{\text{Wann}} = \sum_{R} e^{R} \langle W_{\text{mo}}|\mathcal{T}_{\alpha}|W_{\text{mR}} \rangle,
\]

where \( |W_{\text{mR}} \rangle \) are the MLWFs and matrix elements in the basis of MLWFs, such as \( \langle W_{\text{mo}}|\mathcal{T}_{\alpha}|W_{\text{mR}} \rangle \), need to be computed before the final Wannier interpolation step, which uses a 1024\times1024 Monkhorst-Pack \( k \)-mesh in order to converge the linear response coefficients accurately.

For the calculation of the induced ISOT current on the atomic scale we define the layer-resolved velocity operator

\[
v_{\text{Wann}}(L) = v_{\text{Wann}}(n(L)) \delta_{m(L)},
\]
where $\theta_m(L) = 1$ if MLWF orbital $m$ belongs to layer $L$ and zero otherwise. Here, each MLWF is attributed to the one atomic layer to which it is closest. Replacing $v_a$ in Eq. (56) by $v_a(L)$ allows us to compute the contribution of layer $L$ to the induced ISOT current.

Additionally, we define the layer-resolved spin current density operator $Q_a(L)$ for spin currents flowing in $z$ direction by

$$\langle \psi_{\omega} | Q_a(L) | \psi_{\omega m} \rangle = \frac{1}{A} \int_{S_L} dS \cdot \langle \psi_{\omega} | Q_a(r) | \psi_{\omega m} \rangle,$$  \hspace{1cm} (59)

where the integration is over the boundary $S_L$ between layers $L - 1$ and $L$, $A$ is the $xy$ cross sectional area of the unit cell, and

$$Q_a(r) = \frac{\hbar}{2 i m} \left[ \delta(r - \bar{r}) \nabla - \nabla \delta(r - \bar{r}) \right] J_z,$$  \hspace{1cm} (60)

is the spin current density operator at point $r$. By replacing in Eq. (5) the current density operator $-e v_a/V$ by $Q_a(L)$, we can determine the spin current profile in Pt:

$$Q_a(L, t) = \frac{1}{A} \sum_\beta w_{\beta a}(L, \dot{M}(t)) \left[ \dot{M}(t) \times \frac{d\dot{M}(t)}{dt} \right]_\beta,$$  \hspace{1cm} (61)

where we defined

$$w_{\beta a}(L, \dot{M}) = -A \lim_{\omega \to 0} \frac{\text{Im} G_{Q_a,L,\beta}^R(h\omega, \dot{M})}{\hbar \omega}.$$  \hspace{1cm} (62)

With the Fourier transform of the retarded spin-current torque correlation function

$$G_{Q_a,L,\beta}^R(h\omega, \dot{M}) = -i \int_0^\infty dt e^{i \omega t} \left\{ \langle [Q_a(L), \mathcal{T}_\beta](-t) \rangle - \langle [Q_a(L), \mathcal{T}_\beta(t)] \rangle \right\}.$$  \hspace{1cm} (63)

Within the independent particle approximation Eq. (62) becomes

$$w_{\beta a}(L) = w_{\beta a}^{(1)}(L) + w_{\beta a}^{(1b)}(L) + w_{\beta a}^{(1b)}(L),$$

with

$$w_{\beta a}^{(1)}(L) = \frac{eA}{Nh} \sum_k \text{Tr} \left( Q_a(L) G_k^R(E_F) \mathcal{T}_\beta G_k^R(E_F) \right),$$

$$w_{\beta a}^{(1b)}(L) = -\frac{eA}{Nh} \text{Re} \text{Tr} \left( Q_a(L) G_k^R(E_F) \mathcal{T}_\beta G_k^R(E_F) \right),$$

$$w_{\beta a}^{(1b)}(L) = \frac{eA}{Nh} \sum_k \int_{-\infty}^{E_F} dE \text{Re} \text{Tr} \left( Q_a(L) G_k^R(E) \mathcal{T}_\beta G_k^R(E) \right) \frac{dG_k^R(E)}{dE}$$

$$- Q_a(L) \frac{dG_k^R(E)}{dE} \mathcal{T}_\beta G_k^R(E) \right).$$

where we suppressed the $\dot{M}$ dependence for notational convenience.

In the case of the SHE contribution to SOT, spin currents are generated by the applied electric field rather than spin pumping. Nevertheless, similar decay properties of currents and spin currents are expected in this case due to reciprocity of the SHE/ISHE-mediated contributions to SOT and ISOT.

![FIG. 1: Layer-resolved ISOT current $I_{\text{even}}^{\text{even}}(L)$ induced in Co(3)/Pt(20) by magnetization dynamics. The total ISOT current is $I_{\text{even}} = \sum L I_{\text{even}}^{\text{even}}(L)$. The relative contributions of the layers, i.e., $I_{\text{even}}^{\text{even}}(L) / I_{\text{even}}$, is shown for two values of broadening, $\Gamma = 25$ meV and $\Gamma = 100$ meV. Solid line: Exponential fit according to Eq. (68).](image)

order to investigate spin currents in the SOT case, we define the coefficients

$$q_{\alpha a}(L, \dot{M}) = A e \lim_{\omega \to 0} \frac{\text{Im} G_{Q_a,L,\alpha}^R(h\omega, \dot{M})}{\hbar \omega}.$$  \hspace{1cm} (64)

For example, $q_{\alpha a}(L)$ quantifies the linear response of spin currents flowing in $z$ direction with spin pointing in $y$ direction to the electric field in $x$ direction. Within the independent particle approximation $q_{\alpha a}(L)$ is expressed similarly to the torkance (Eq. (56)): Only $T_{\omega}$ has to be replaced by $-AQ_a(L)$ in the expressions.

### B. Even SOT and ISOT

We first discuss the even SOT and ISOT (see Eq. (16) for the definition). The odd components are discussed in Sec. [V.C]

At $\Gamma = 25$ meV we obtain a torkance of $t_{\text{even}}^{xy,25\text{meV}} = 0.68$ $e\alpha_0$ per unit cell, where $e\alpha_0$ is the atomic unit of torkance, which amounts to $e\alpha_0 = 8.478 \cdot 10^{-30}$ Cm. A slightly smaller value of $t_{\text{even}}^{xy,100\text{meV}} = 0.53$ $e\alpha_0$ is obtained at $\Gamma = 100$ meV. Similar values for the torkance in Co/Pt(111) were reported for different thicknesses of Pt. Dividing these torkances by the magnetic moment per unit cell of $\mu = 5.78 \mu_B$ we obtain the effective fields per applied electric field of $t_{\text{even}}^{xy,25\text{meV}} / \mu = 0.011$ mT/cm/V and $t_{\text{even}}^{xy,100\text{meV}} / \mu = 0.0084$ mT/cm/V.

When the magnetization precesses in a circular orbit around the $z$ axis in the small-cone limit the current density

$$I_{\text{even}}^{xy,25\text{meV}}(t) = -8\gamma \frac{P a_s}{m} \sin(\theta) \sin(\omega t),$$

$$I_{\text{even}}^{xy,100\text{meV}}(t) = -68\gamma \frac{P a_s}{m} \sin(\theta) \sin(\omega t)$$  \hspace{1cm} (66)

is induced due to the even torkance $t_{\text{even}}^{xy}$ according to Eq. (22), where we used $A_0 = t_{\text{even}}^{xy}$ and $A = 23.8 \alpha_0$. The current $I_{\text{even}}^{xy}(t)$ arises dominantly from the combination of spin pumping and ISHE. As discussed in Sec. [III.B] the layer-resolved spin current profile is expected to reflect the spatial decay of the spin current pumped into the Pt layer. Replacing $v_a$ in Eq. (56) by $v_a(L)$ (Eq. (58)) yields the current distribution shown in Fig. [1]. In the Pt layer, the layer-resolved induced current is well
described by an exponential function,

\[ I_{x, \text{even}}(z) = I_{x, \text{even}}(z_{20}) e^{(z - z_{20})/\lambda_{\text{ISOT,1}}}, \]  

(67)

where \( z_{20} \) is the \( z \) coordinate of layer Pt20. Fitting Eq. (67) to the \( I_{x, \text{even}}(L) \) profile obtained from first principles yields \( \lambda_{\text{ISOT,1}} = 0.58 \) nm and \( \lambda_{\text{ISOT,2}} = 0.70 \) nm.

The component \( w_{yy} \), which is defined in Eq. (64), describes spin current in phase with \( I_{x, \text{even}}(t) \) and with spin pointing in \( y \) direction. Within Pt, the \( L \)-dependence of \( w_{yy} \), shown in Fig. 2 is approximately given by

\[ w_{yy}(z) = 0.087 e^{(z - z_{20})/\lambda_{\text{ISOT,2}}}, \]  

(68)

where \( \lambda_{\text{ISOT,2}} = 0.89 \) nm. At smaller broadening \( \Gamma = 25 \) meV, our numerical results deviate too much from the exponential behavior to use Eq. (68) for fitting. The ISOT currents shown in Fig. 1 decay faster in Pt than the spin currents described by \( w_{yy} \). Thus, Eq. (64), which predicts spin current and ISHE-current to be proportional, is not exactly satisfied, in particular not at \( \Gamma = 25 \) meV, where the spin current decay is not well-described by an exponential. However, Eq. (64) is approximately satisfied at \( \Gamma = 100 \) meV, where both the ISOT current and the pumped spin current decay exponentially with \( \lambda_{\text{ISOT,1}} \approx \lambda_{\text{ISOT,2}} \). The small difference \( \lambda_{\text{ISOT,2}} - \lambda_{\text{ISOT,1}} = 0.19 \) nm amounts to less than one Pt interlayer distance.

As a consequence of the violation of Eq. (64), extraction of \( \gamma_{\text{ISHE}} \) on the basis of layer-resolved ISOT current \( I_{x, \text{even}}(L) \) and layer-resolved spin current leads to an \( L \)-dependence of \( \gamma_{\text{ISHE}} \), in particular in the \( \Gamma = 25 \) meV case. We obtain \( \tan \gamma_{\text{ISHE}}(L = \text{Pt20}) = 0.27 \) and \( \tan \gamma_{\text{ISHE}}(L = \text{Pt20}) = 0.16 \). Since the ISOT charge current decays faster in Pt than the spin current, these values constitute the maxima of the layer-resolved ISHE-angles in Pt.

Comparison of Eq. (61) and Eq. (64) yields an expression for the spin mixing conductance:

\[ \text{Reg}^{11} = \frac{4\pi}{hA} w_{yy} (L = \text{Co1}), \]  

(69)

where \( w_{yy} (L = \text{Co1}) \) is proportional to spin current flowing between the layers Pt20 and Co1. We obtain \( \text{Reg}^{11} \) \( 100 \) meV \( = 1.8 \cdot 10^{19} \) m\(^{-2}\) and for \( \Gamma = 100 \) meV a slightly larger value.

\[ 25 \text{ meV} \quad \text{and} \quad 100 \text{ meV} \quad \text{(fit)} \]

\[ 100 \text{ meV} \quad \text{fit} \]

FIG. 2: Layer-resolved spin current induced by magnetization dynamics for two values of broadening, \( \Gamma = 25 \) meV and \( \Gamma = 100 \) meV. The coefficient \( w_{yy} \) describes spin current flowing in \( z \) direction with spin pointing in \( y \) direction and in phase with \( I_{x, \text{even}}(t) \). Solid line: Fit according to Eq. (68).

\[ \frac{\text{Re}^{11}}{100 \text{meV}} = 2.0 \cdot 10^{19} \text{ m}^{-2}. \]

It has been shown recently\(^2\) that \( \text{Re}^{11} \) in Co/Pt arises almost entirely from the spin-flux into the Co-layer. Thus, the above extraction of \( \text{Re}^{11} \) from \( w_{yy} \) is meaningful in this case despite the presence of spin-orbit interaction in the calculation.

We now turn to the SHE contribution to the even SOT. In this case, spin currents are generated by the applied electric field rather than spin pumping, but we expect similar decay properties of currents and spin currents due to reciprocity of the SHE/ISHE-mediated contributions to SOT and ISOT. In Fig. 3 we show the linear response coefficients of the layer-resolved spin current \( q_{yx}^{\text{even}}(L) \) as diamonds for two values of broadening, \( \Gamma = 25 \) meV and \( \Gamma = 100 \) meV (see Eq. (65) for the definition of \( q_{yx}^{\text{even}}(L) \)). Evaluating the SHE-to-SOT conversion efficiency defined in Eq. (50) from the ratio of torque to maximal spin current we obtain \( \xi_{\text{25meV}} = \frac{q_{yx}^{\text{even}}(L = \text{Pt11})}{q_{yx}^{\text{even}}(L = \text{Pt11})} = 0.74 \). At \( \Gamma = 100 \) meV the value is slightly lower: \( \xi_{\text{100meV}} = 0.57 \). We can roughly understand the value of \( \xi_{\text{100meV}} \) from the decay of spin current discussed in Eq. (68). We assume that each Pt layer is the source of a spin current \( \tilde{Q}_{x}^{L} \), which decays exponentially with increasing distance from the layer, i.e., the Pt layer \( L \), which is located at \( z_{L} \), provides the contribution

\[ \tilde{Q}_{x}^{L}(z) = \tilde{Q}_{x,\text{max}}^{L} e^{-kz/\lambda_{\text{ISOT,2}}}, \]  

(70)

to the spin-current profile. The spin current due to SHE at the center of a sufficiently thick Pt layer is then given by

\[ \tilde{Q}_{x}^{\text{center}} \approx \frac{\tilde{Q}_{x,\text{max}}^{L}}{d} \int_{-\infty}^{\infty} d z e^{-kz/\lambda_{\text{ISOT,2}}} = \frac{2\lambda_{\text{ISOT,2}} \tilde{Q}_{x,\text{max}}^{L}}{d}, \]  

(71)

where \( d \) is the interlayer distance and we assumed \( \tilde{Q}_{x,\text{max}}^{L} \) to be independent of \( L \), i.e., \( \tilde{Q}_{x,\text{max}}^{L} = \tilde{Q}_{x,\text{max}}^{\text{even}} \). The spin current maximally available to penetrate through the Co/Pt interface and to produce a torque on the Co magnetization is only half.
of $Q_y$, 

$$Q_{y,\text{interface}} \approx \frac{Q_{y,\text{interface}}}{d} \int_{-\infty}^{0} dz e^{-\alpha_i \lambda_{\text{SOT},2}} = \lambda_{\text{SOT},2} \frac{Q_{y,\text{max}}}{d},$$  

(72)

because only the half space $z < z_{\text{Co1}}$ provides spin current that could enter through the interface. Thus, $\xi \approx Q_{y,\text{interface}}/Q_{y,\text{center}} \approx 0.5$. Hence, the model Eq. (70) explains rather well our finding of $\xi_{100\text{meV}} = 0.57$. At the smaller broadening $\Gamma = 25 \text{ meV}$ the model Eq. (70) is not applicable because the spin current decay is not exponential, as shown in Fig. (4).

Computing the electric conductivities based on the same formalism as used for SOT and ISOT, we obtain $\sigma_{xx}^{100\text{meV}} = 1.2 \cdot 10^7 \text{ S/m}$ and $\sigma_{xy}^{100\text{meV}} = 0.34 \cdot 10^7 \text{ S/m}$. From these conductivities and the spin currents at the center of Pt, which are described by $q_{xx}^{\text{even}}(L = \text{Pt11})$, we obtain the following SHE angles: $\tan \gamma_{\text{SHE}}^{100\text{meV}} = 0.029$ and $\tan \gamma_{\text{SHE}}^{100\text{meV}} = 0.109$. These SHE angles are smaller than the corresponding ISHE angles given above. In Sec. [10] we argue that $\tan \gamma_{\text{SHE}} < \tan \gamma_{\text{ISHE}}$ is expected in the presence of strong extrinsic spin scattering. However, extrinsic spin scattering is not present in the constant $\Gamma$ approximation used in this work to describe disorder. Hence, we attribute the difference between the angles $\gamma_{\text{SHE}}$ and $\gamma_{\text{ISHE}}$ to an enhancement of SHE close to the Co/Pt interface: We determined $\gamma_{\text{SHE}}$ at the center of the Pt layer, but $\gamma_{\text{SHE}}$ close to the Co/Pt interface. Thus, $Q_{y,max}$ in the model Eq. (70) is not constant but increases as $L$ approaches the Co/Pt interface.

At $\Gamma = 100 \text{ meV}$ the spin current in the region between Pt12 and Co1 is well-described by the exponential fit

$$q_{xx}^{\text{even}}(z) = \left[0.97 - 0.35 e^{-(z-x_{\text{Pt11}})/100\text{meV}}\right] e\alpha_0, \quad (73)$$

with $\lambda_{\text{SOT},3}^{100\text{meV}} = 0.46 \text{ nm}$. Clearly, $\lambda_{\text{SOT},2}^{100\text{meV}}$ is significantly longer. We attribute the difference between the lengths $\lambda_{\text{SOT},3}^{100\text{meV}}$ and $\lambda_{\text{SOT},2}^{100\text{meV}}$ to the $L$-dependence of $Q_{y,max}$ in the model Eq. (70), i.e., we assume that close to surfaces and interfaces $Q_{y,max}$ introduces an additional length scale. In the region from Pt1 to Pt10 the spin current is approximately given by

$$q_{xx}^{\text{even}}(z) = \left[0.92 - 0.63 e^{-(z-x_{\text{Pt10}})/100\text{meV}}\right] e\alpha_0, \quad (74)$$

with $\lambda_{\text{SOT},4}^{100\text{meV}} = 0.32 \text{ nm}$. The similarity of lengths $\lambda_{\text{SOT},3}^{100\text{meV}} \approx \lambda_{\text{SOT},4}^{100\text{meV}}$ means that the $L$-dependence of $Q_{y,max}$ at the surface of Pt is similar to the one at the Co/Pt interface. At the smaller broadening of $\Gamma = 25 \text{ meV}$ we find $\lambda_{\text{SOT},2}^{100\text{meV}} = 0.15 \text{ nm}$, but due to oscillations the first principles data are less well-described by the exponential fit.

An interesting question concerns the influence of the vacuum boundary on the value of $\lambda_{\text{SOT},4}^{100\text{meV}}$. In order to shed light on this question it is necessary to inject SHE spin current directly into Pt away from vacuum boundaries and without employing spin pumping through the Co/Pt interface. For this purpose we divide the Pt layer into two regions: In the atomic layers Pt1 through Pt12 we switch off the mechanical force $-eE$ that the electrons would otherwise experience due to the applied electric field $E$. Only the atomic layers Pt13 through Co3 are subject to the mechanical force $-eE$ in this modified calculation. Thus, only Pt13 through Pt20 generate sizable SHE spin current (SHE in Co is small). Noting that the mechanical force is represented in Eq. (55) by the velocity operator, we define the modified velocity operator

$$\bar{v}_{\text{ann}}(L) = v_{\text{ann}} \sum_{L_1 \leq L \leq L_2} \theta_i(L_1)\theta_i(L_2), \quad (75)$$

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$$\bar{v}_{\text{ann}}(L) = v_{\text{ann}} \sum_{L_1 \leq L \leq L_2} \theta_i(L_1)\theta_i(L_2), \quad (75)$$

In Fig. (4) we show the layer-resolved even torkance, i.e., the linear-response coefficient of the torque acting on the magnetization of a given layer, and the linear-response coefficient
resolved torkances and spin fluxes coincide approximately. Indeed this is the case, as illustrated in Fig. 5 which shows the torkance as a function of the region with mechanical force set to zero. If the mechanical force is switched off in all Pt layers and only active in the Co layers (data points at L=Co1), t\text{even} is very small because the even torque arises dominantly from the SHE in Pt which is switched off when the mechanical force is set to zero. For L=Pt1 through Co1, the torkance is approximately given by

$$t_{yx}^\text{even}(z) = [0.65 - 0.68e^{-(z_{\text{Co1}}-z)/\lambda_{\text{SOT,1}}}]e_0,$$

where the mechanical force is set to zero from Pt1 through layer L−1 and $\lambda_{\text{SOT,1}} = 100\text{ meV}$. We find a weak $\lambda$-dependence: $\lambda_{\text{SOT,1}} = 0.71\text{ nm}$. As expected, $\lambda_{\text{SOT,1}} \approx \lambda_{\text{SOT,1}}$, where $\lambda_{\text{SOT,1}}$ is discussed above, below Eq. (67).

We find $\lambda_{\text{SOT,3}} < \lambda_{\text{SOT,1}} < \lambda_{\text{SOT,2}}$, i.e., the effective length scale $\lambda_{\text{SOT,1}}$ is a mixture of $\lambda_{\text{SOT,2}}$ and $\lambda_{\text{SOT,3}}$. The contribution of Pt layers sufficiently far from the Co/Pt interface to $t_{yx}^\text{even}$ is limited by the decay length $\lambda_{\text{SOT,2}}$ of spin current that they emit towards the Co layer. However, close to the interface with Co, $Q_L^{\text{SOT}}$ in Eq. (70) becomes L-dependent, whereby the length $\lambda_{\text{SOT,3}}$ is admixed.

The lengths $\lambda_{\text{SOT,2}}$ and $\lambda_{\text{SOT,3}}$ determine also the Pt layer-thickness dependence of SOT: The SHE current back-reflected from the Pt surface at Pt1 and opposite in sign to the primary SHE current decays on the scale of $\lambda_{\text{SOT,2}}$. At the same time, according to the model Eq. (70), in thin Pt layers with thicknesses smaller than $\lambda_{\text{SOT,2}}$ the primary SHE spin current itself is suppressed, because $\lambda_{\text{SOT,2}}$ determines the length scale on which the spin current increases due to the addition of the contributions Eq. (70) from several atomic layers before saturation is reached due to the exponential decay on the scale of $\lambda_{\text{SOT,2}}$. Finally, $Q_L^{\text{SOT}}_{\text{max}}$ in Eq. (70) is L-dependent on the length scale of $\lambda_{\text{SOT,3}}$ close to the Pt surface and the Co/Pt interface. In order to investigate the Pt-thickness dependence, we performed additional calculations of the torkance for Pt layer thicknesses of 2, 7, 10, 13 and 15 atomic layers, which correspond to 0.45 nm, 1.6 nm, 2.3 nm, 3.0 nm and 3.4 nm, respectively. Atomic coordinates and computational parameters were chosen as discussed above for Co(3)/Pt(20).

The obtained torkances $t_{yx}^\text{even}$ are shown in Fig. 6 for broadenings of $\Gamma = 5$ meV and 100 meV. $t_{yx}^\text{even}$ is suppressed at smaller Pt thicknesses. Since $t_{yx}^\text{even}$ determines both the even part of SOT (according to Eq. (8)) and the even part of ISOT (according to Eq. (16)), the suppression of $t_{yx}^\text{even}$ at smaller thicknesses occurs for both SOT and ISOT. Rather than developing an involved model in terms of $\lambda_{\text{SOT,2}}$ and $\lambda_{\text{SOT,3}}$ one...
can describe the Pt-thickness dependence in terms of a single effective length. For this purpose, experimental data of the ISHE current measured in bilayers under FMR are usually fitted with \( \tan(\frac{D}{L}) \), where \( D \) is the thickness of the NM layer.\(^\text{25}\)

Using the same model,

\[
t_{\text{yy}}^{\text{even}}(D) = 0.51 \tanh \left( \frac{D}{2 \lambda_{\text{D}}^\text{100meV}} \right) ea_0,
\]

(80)

to fit our first principles results yields \( \lambda_{\text{D}}^\text{100meV} = 0.6 \text{ nm} \) and \( \lambda_{\text{D}}^\text{25meV} = 0.55 \text{ nm} \). As expected, we find \( \lambda_{\text{SOT},3}^{\text{odd}} < \lambda_{\text{D}} < \lambda_{\text{SOT},3}^{\text{odd}} \). Similarly short but slightly longer length scales of roughly \( 1.5 \text{ nm} \) have been observed in Pt in recent experiments.\(^\text{13},\text{29},\text{31},\text{52}\)

All exponential fits in this section as well as the tanh fit in Eq. (80) match the first principles data well at the elevated broadening of \( \Gamma = 100 \text{ meV} \), but less so at the smaller broadening of \( \Gamma = 25 \text{ meV} \). The oscillatory deviations from the fits reflect the quantum confinement in the out-of-plane direction. These oscillations, which are clearly visible at \( \Gamma = 25 \text{ meV} \) in the theoretical thickness dependence depicted in Fig. 6, are expected to be observable also experimentally in epitaxially grown magnetic bilayers.

C. Odd SOT and ISOT

We obtain torkances per unit cell of \( t_{xx}^{\text{odd}} = 0.17 ea_0 \) and \( t_{xx}^{\text{odd}} = 0.15 ea_0 \) at broadening of \( \Gamma = 25 \text{ meV} \) and \( \Gamma = 100 \text{ meV} \), respectively. Dividing these torkances by the magnetic moment per unit cell of \( \mu = 5.78 \mu_B \) we obtain the effective fields per applied electric field of \( t_{xx}^{\text{odd}}/\mu = 0.0027 \text{ mTcm/V} \) and \( t_{xx}^{\text{odd}}/\mu = 0.0024 \text{ mTcm/V} \). According to Eq. (22) the current density

\[
\frac{I_{xx}^{\text{odd}}(t)}{\ell \omega} = \frac{22 \text{ pA}}{\text{m}} \sin(\theta) \cos(\omega t),
\]

\[
\frac{I_{xx}^{\text{odd}}(t)}{\ell \omega} = \frac{19 \text{ pA}}{\text{m}} \sin(\theta) \cos(\omega t),
\]

(81)

is induced due to \( t_{xx}^{\text{odd}} \) when the magnetization precesses around the \( z \) axis in the small-cone limit. Here, we used \( C_0 = t_{xx}^{\text{odd}} \) and \( \ell = 23.8 a_0^2 \). This contribution from \( t_{xx}^{\text{odd}} \) is thus \( -90^\circ \) phase shifted with respect to the contribution from \( t_{xx}^{\text{even}} \) given in Eq. (66), i.e., it lags behind by a quarter period.

In Fig. 7 we show the odd torkance as a function of the region with mechanical force switched off. If the mechanical force is switched off for Pt1 through Pt20 such that only the layers Co1, Co2 and Co3 are subject to it (see the data points at \( L = \text{Co1 in the figure} \)), the corresponding odd torque is not very different from the one with the mechanical force switched on everywhere (see the data points at \( L = \text{Pt1 in the figure} \)). To produce a sizable odd torque in Co(3)/Pt(20) it is therefore not crucial to switch on the mechanical force in the Pt layers but it suffices to apply this perturbation to the Co states. As a combined effect of broken inversion symmetry and spin-orbit coupling the spin of a given wave function

\( n \) is correlated with the velocity \( v_{\text{kmn}} \). As a result, the non-equilibrium spin density induced by an applied electric field combined with the exchange interaction gives rise to the odd component of the torkance.\(^\text{9,10,54}\) Application of the mechanical force to Co, i.e., perturbation of the system via the velocity operator within the Co layer, produces therefore the dominant part of nonequilibrium spin density from which the odd torque arises in Co(3)/Pt(20). This stands in marked contrast to the even torque in this system, which is mainly driven by SHE from Pt and thus very small if the mechanical force is turned off in all Pt layers, as shown in Fig. 8. If the mechanical force is applied only to layers Co2 and Co3 (see data points at \( L = \text{Co2 in the figure} \)) the resulting torkance is much smaller compared to the situation where all three Co layers are subject to it. Thus, the perturbation of the Co1 layer by the mechanical force is essential.

We thus expect that the ISOT current induced by magnetization dynamics flows mainly in the Co1 layer. This is indeed the case, as Fig. 8 shows. In particular, at \( \Gamma = 100 \text{ meV} \) the currents flowing in Co2, Co3 and the Pt layer are almost negligible. At the smaller broadening \( \Gamma = 25 \text{ meV} \) the induced currents in Co2, Co3 and Pt are larger, especially in the Co2 and Co3 layers.

In Fig. 9 the layer-resolved odd torkance and the linear-
response coefficient of spin flux into layer $L$, i.e.,

$$\Delta q_{xx}^{\text{odd}}(L) = q_{xx}^{\text{odd}}(L) - q_{xx}^{\text{odd}}(L + 1), \quad (82)$$

are shown for two values of broadening, $\Gamma = 25$ meV and $\Gamma = 100$ meV. For the layers Co1 through Co3 the layer-resolved torques coincide approximately with the spin fluxes like in the case of the even torque. For $\Gamma = 100$ meV the magnetization of layer Pt20 experiences a torque of 0.085$ea_0$. At the same time there is a spin flux out of layer Pt20 characterized by the coefficient $-\Delta q_{xx}^{\text{odd}}(L = \text{Pt20}) = 0.087e a_0$. This spin flux is transferred to the Co layer where it exerts a torque on the Co magnetization. The sum of torque and spin flux coefficient of Pt20 amounts to 0.172$ea_0$ and approximately accounts for the total odd torque of 0.15$ea_0$ at $\Gamma = 100$ meV. The angular momentum that gives rise to the torque on the magnetization is thus picked up from the lattice at Pt20 and roughly 50% of it is directly transferred to the magnetization of the Pt20 layer while the rest is transported to the Co layer via spin current. Above we have shown that the mechanical force on the Co1 layer is crucial to produce a sizable odd torque. Since the pick-up of angular momentum from the lattice by the spin system happens in Pt20, the hybridization of the Co1 states with the Pt20 states is thus essential.

While the total odd torque does not differ a lot between the $\Gamma = 25$ meV and $\Gamma = 100$ meV cases, the maximum of the layer resolved odd torque and spin flux, which is attained on Co1, decreases by roughly a factor of three when the broadening is increased from $\Gamma = 25$ meV to $\Gamma = 100$ meV. This decrease does not manifest itself in the total odd torque because the torques and spin fluxes on Co2 are opposite in sign to the ones on Co1 and the amplitude of torque and spin flux on Co2 decreases also as the broadening is increased.

V. SUMMARY

SOT and ISOT are reciprocal effects. Both of them can be expressed conveniently in terms of the torque tensor $t(\hat{M})$, which depends on the magnetization direction $\hat{M}$. In the case of the SOT phenomenon, the torque $T(\hat{M})$ on the magnetization due to the application of an electric field $E$ is given by $T(\hat{M}) = t(\hat{M})E$. If $\hat{M}$ changes as a function of time, the reciprocal effect, the ISOT, can be observed. It consists in the generation of a current density $j(t) = [t(\hat{M}(t))]T[\hat{M}(t) \times \frac{d\hat{M}(t)}{dt}]/V$, where $V$ is the unit cell volume. On the basis of this reciprocity relation and recent experimental results for the SOT in bilayer systems, we predict the angular dependence of the FMR-driven ISOT in bilayers. We find that measurements of the dc voltage associated with the FMR-driven ISOT are insufficient to determine $t(\hat{M})$ in general and that additionally the ac voltage needs to be measured phase-sensitive to determine $t(\hat{M})$ completely. From the reciprocity between SOT and ISOT it follows that the presence of ISHE limits the spatial decay length of spin currents. Furthermore, the presence of additional spin relaxation via spin flip scattering requires SHE and ISHE angles to differ. Within the Kubo linear response formalism we investigate SOTs and ISOTs in Co/Pt(111) magnetic bilayers using the electronic structure provided from first principles density functional theory. Magnetization-dynamics induced charge currents and spin currents are resolved on the atomic scale to extract model parameters and to expose the mechanisms underlying the ISOT. Likewise the spin currents accompanying the SOT are resolved on the atomic scale for the same purposes. It is found that several different effective lengths govern the position-dependence of these various currents and that SHE and ISHE are modified close to interfaces and surfaces. Comparison of the various currents accompanying SOT on the one hand and ISOT on the other hand highlight the reciprocity of the two phenomena on the microscopic scale.

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