Spin-Flip Scattering Effect on the Current-Induced Spin Torque in Ferromagnet-Insulator-Ferromagnet Tunnel Junctions

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Abstract

We have investigated the current-induced spin transfer torque of a ferromagnet-insulator-ferromagnet tunnel junction by taking the spin-flip scatterings into account. It is found that the spin-flip scattering can induce an additional spin torque, enhancing the maximum of the spin torque and giving rise to an angular shift compared to the case when the spin-flip scatterings are neglected. The effects of the molecular fields of the left and right ferromagnets on the spin torque are also studied. It is found that $\tau_{Rx}/I_e$ ($\tau_{Rx}$ is the spin-transfer torque acting on the right ferromagnet and $I_e$ is the tunneling electrical current) does vary with the molecular fields. At two certain angles, $\tau_{Rx}/I_e$ is independent of the molecular field of the right ferromagnet, resulting in two crossing points in the curve of $\tau_{Rx}/I_e$ versus the relevant orientation for different molecular fields.

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The spin-polarized transport in multilayer structures exhibits new effects such as the giant magnetoresistance [1] (GMR), the spin transfer effect [2], and so on. How to use the spin degree of freedom of electrons in ferromagnetic materials to construct new devices is at present a focus in the field of spintronics. Spin-polarized electrons flowing from one ferromagnetic layer into another layer in which the molecular field deviates by an angle may transfer the angular momentum to the local angular momentum of the ferromagnetic layer, thereby exerting a torque on the magnetic moments (see e.g. Refs. [2–9]). This phenomenon is usually called the spin transfer effect [2]. The torques in the plane spanned by $\mathbf{s}_1$ and $\mathbf{s}_2$, where $\mathbf{s}_1$ and $\mathbf{s}_2$ are spin moments in the left and right ferromagnets, are normally called the dynamic nonequilibrium spin torques [9]. Spin transfer motion of $\mathbf{s}_1$ and $\mathbf{s}_2$ within their spanned plane is different from the spin precession like $\partial \mathbf{s}_1/\partial t = \hbar J \mathbf{s}_1 \times \mathbf{s}_2$ out of the spanned plane which describes the conventional exchange coupling [12,13]. Therefore, the spin transfer effect causes new physical phenomena in magnetic multilayer structures. When the current is large enough, it could switch the magnetic states of the local angular momentum. Such a current-induced change of the magnetic state has been observed in several experiments (see e.g. Refs. [4–7]). As a result, the spin transfer effect may provide a mechanism for a current-controlled magnetic memory element. To deal with the spin transfer effect, it is useful to introduce the concepts such as the spin current and the spin torque to describe the coupling between the conduction electrons and the magnetic moments of ferromagnetic materials. These concepts are first proposed by Slonczewski [3] based on a quantum-mechanical model for ferromagnet-insulator-ferromagnet (FM-I-FM) junctions. Then, the concepts are extended to the structures such as ferromagnet-normal metal-ferromagnet (FM-NM-FM) junctions [8,9], ferromagnet-superconductor-ferromagnet junctions [10], and trilayer FM-NM-FM which contacts an normal metal lead or a superconductor lead [11,12], etc., showing that the investigation on spin torques in magnetic junctions has been receiving much attention.

Many works concerning the spin torque are presented for FM-NM-FM structures so far. The work for FM-I-FM structures is still sparse. In particular, when electrons tunnel through
the insulator barrier, the spin-flip scattering may occur [14,15]. The spin-flip electrons feel a
different torque with respect to those non-flip electrons, and could exert an additional
torque to the ferromagnet. Consequently, this additional torque induced by the spin-flip
electrons may play a role as the dynamic spin transfer torque. In this paper, we shall use
the nonequilibrium Green function technique [16] to investigate the spin-flip scattering effect
on the current-induced spin transfer torque in FM-I-FM tunnel junctions.

The system under interest is composed of two ferromagnets which are stretched
to infinite separated by a thin insulator, as illustrated in Fig.1. The molecular field
in the left ferromagnet is assumed to align along the z axis which is in the junction
plane, while the orientation of the molecular field in the right ferromagnet, along
the z' axis, deviates the z axis by an angle θ. The electrons flow along the x
axis which is perpendicular to the junction plane. The Hamiltonian of the system is

\[ H = H_L + H_R + H_T, \]

with

\[ H_L = \sum_{k\sigma} \varepsilon_{k\sigma}^L a_{k\sigma}^\dagger a_{k\sigma}, \]

\[ H_R = \sum_{q\sigma} [ (\varepsilon_R(q) - \sigma M_2 \cos \theta) c_{q\sigma}^\dagger c_{q\sigma} - M_2 \sin \theta c_{q\sigma}^\dagger c_{q\sigma}^\dagger], \]

\[ H_T = \sum_{kq\sigma\sigma'} [ T_{kq}^{\sigma\sigma'} a_{k\sigma}^\dagger c_{q\sigma'} + T_{kq}^{\sigma'\sigma} c_{q\sigma'}^\dagger a_{k\sigma}^\dagger], \]

where \( a_{k\sigma} \) and \( c_{k\sigma} \) are annihilation operators of electrons with momentum \( k \) and spin \( \sigma \)
\((= \pm 1)\) in the left and right ferromagnets, respectively, \( \varepsilon_{k\sigma}^L = \varepsilon_L(k) - eV - \sigma M_1, \) \( M_1 = \frac{a\mu_B h}{2}, \)
\( M_2 = \frac{g\mu_B h}{2}, \) \( g \) is the Landé factor, \( \mu_B \) is the Bohr magneton, \( h_{L(R)} \) is the molecular field of
the left (right) ferromagnet, \( \varepsilon_{L(R)}(k) \) is the single-particle dispersion of the left (right) FM
electrode, \( V \) is the applied bias voltage, \( T_{kq}^{\sigma\sigma'} \) denotes the spin and momentum dependent
tunneling amplitude through the insulating barrier. Note that the spin-flip scattering is
included in \( H_T \) when \( \sigma' = \bar{\sigma} = -\sigma. \) It is this term that violates the spin conservation in the
tunneling process.
With the system defined above, let us now consider the spin torques exerting on the magnetic moments in the right FM electrode of this magnetic tunnel junction. The spin torques, namely the time evolution rate of the total spin of the left or the right ferromagnet, can be obtained by \( \frac{\partial}{\partial t} \langle s_{1,2}(t) \rangle = -\frac{i}{\hbar} \langle [H, s_{1,2}(t)] \rangle \). In Refs. [9,11], the spin torques are defined by considering the momentum conservation \( \partial s_1/\partial t = I(\infty) - I(0) \) [2], where \( I \) is the spin current (whose definition can be found in Refs. [12,8]). Because there are the spin-dependent scatterings caused by the local exchange field inside the ferromagnets, the spin current is no longer conserved inside the ferromagnets. Whereas the total spin is conserved, the lost spin current is transferred to the local magnetic moments, thereby giving rise to a torque exerting on the local magnetic moments of the ferromagnets. So the nonconservation of the nonequilibrium spin current leads to a current-induced nonequilibrium torque [12]. We may consider this issue in another way, i.e. to investigate the evolution rate of the total spin of the ferromagnets. In doing so, one must be cautious to identify the spin-torques implied from the total Hamiltonian. In this model one may see that the right ferromagnet gains two types of torques: one is the equilibrium torque caused by the spin-dependent potential (i.e. the magnetic exchange interaction), and the other is from the electrons tunneling through the insulating barrier from the left side. The latter can be obtained from the tunneling term \( H_T \), which is nothing but the current-induced spin transfer torque in the plane spanned by \( h_L \) and \( h_R \). When the applied bias is absent, the left and right ferromagnets will only undergo the spin torque caused by the spin-dependent potential, and the current-induced torques would not appear. Therefore, we can define the current-induced spin transfer torque as \( \tau = -\frac{i}{\hbar} \langle [H_T, s_2(t)] \rangle \). Note that a similar expression in a current matrix form is introduced in Ref. [10]. The equilibrium torques caused by a spin-dependent potential will not be considered here. The total spin of the right ferromagnet is

\[
\mathbf{s}_2(t) = \frac{\hbar}{2} \sum_{k\mu\nu} c_{k\mu}^{\dagger} c_{k\nu} (R^{-1}_{\mu})^\dagger \hat{\sigma} (R^{-1}_{\nu} \chi_{\nu}),
\]

where \( R = \begin{pmatrix}
\cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\
\sin \frac{\theta}{2} & \cos \frac{\theta}{2}
\end{pmatrix} \), \( \hat{\sigma} \) is Pauli matrices and \( \chi_{\mu(\nu)} \) is spin states. Note that Eq. (3)
is written in the \textit{xyz} coordinate frame while the spins \( s_2 \) are quantized in the \textit{x'y'z'} frame. From \( \dot{s}_{1,2} \sim I_e \hat{s}_{1,2} \times (\hat{s}_1 \times \hat{s}_2) \) with \( I_e \) the electrical current, we can judge that the direction of the spin transfer torque is along \textit{x'} direction in the \textit{x'y'z'} coordinate frame. We can further write the spin transfer torque in Eq.(3) as
\[ s_2(t) = \frac{\hbar}{2} \sum_{kq} \langle c_{kq}^\dagger \cos \theta - \sigma c_{kq}^\dagger c_{kq} \sin \theta \rangle = s_{2x0} \cos \theta - s_{2z0} \sin \theta, \]
where \( s_{2x0} \) and \( s_{2z0} \) are \textit{x'}- and \textit{z'}-components of the total spins in the \textit{x'y'z'} coordinate frame in which the spins \( s_2 \) are quantized. Hence, the current-induced spin transfer torque can be obtained:
\[ \tau_{R \textit{x'}} = - \cos \theta \text{Re} \sum_{kq} \int \frac{d\varepsilon}{2\pi} Tr_\sigma [G^<_{kq}(\varepsilon) \hat{\sigma}^1 T^\dagger] + \sin \theta \text{Re} \sum_{kq} \int \frac{d\varepsilon}{2\pi} Tr_\sigma [G^<_{kq}(\varepsilon) \hat{\sigma}^3 T^\dagger], \]
where \( \hat{\sigma}^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \), \( \hat{\sigma}^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \) are Pauli matrices, \( T = \begin{pmatrix} T_1 & T_2 \\ T_3 & T_4 \end{pmatrix} \) with the elements \( T_i \ (i = 1, ..., 4) \) being the tunneling amplitudes which are for simplicity assumed to be independent of \( k \) and \( q \) (namely, \( T^{\uparrow \uparrow}, T^{\uparrow \downarrow}, T^{\downarrow \uparrow}, T^{\downarrow \downarrow} \) respectively), \( Tr_\sigma \) stands for the trace of the matrix taking over the spin space, and \( G^<_{kq}(\varepsilon) \) is the lesser Green function in spin space defined as
\[ G^<_{kq}(\varepsilon) = \begin{pmatrix} G^{\uparrow \uparrow, <}(\varepsilon) & G^{\uparrow \downarrow, <}(\varepsilon) \\ G^{\downarrow \uparrow, <}(\varepsilon) & G^{\downarrow \downarrow, <}(\varepsilon) \end{pmatrix}, \]
with \( G^{\sigma \sigma', <}(\varepsilon) = \int dt e^{i(\varepsilon-t') \varepsilon} c_{kq}^{\sigma \sigma'}(t-t') \) and \( G^{\sigma \sigma', <}(t-t') \equiv i \langle c_{\sigma'}^\dagger (t') a_{\sigma}(t) \rangle \). By using the nonequilibrium Green function technique [17], we can get the torque, \( \tau_{R \textit{x'}} \), to the first order of the Green function by
\[ \tau_{R \textit{x'}} = \pi \int d\varepsilon [f(\varepsilon + eV) - f(\varepsilon)] Tr_\sigma [\Lambda(\hat{\sigma}^1 \cos \theta - \hat{\sigma}^3 \sin \theta)], \]
where \( f(x) \) is the Fermi function, the matrix \( \Lambda \) is defined as \( \Lambda = T^\dagger D_L(\varepsilon + eV)T^0_R(\varepsilon)R^\dagger \)
\[ = \begin{pmatrix} \Lambda_1 & \Lambda_2 \\ \Lambda_3 & \Lambda_4 \end{pmatrix}, \quad \text{and} \quad D_L(R) = \begin{pmatrix} D_{L(R)^0} & 0 \\ 0 & D_{L(R)^\dagger} \end{pmatrix} \]
whose elements \( D_{L(R)^0} = D_{L(R)}(\varepsilon \pm M_1(2)) \) are the density of states (DOS) of electrons with spin up and down in the left (right) ferromagnet, respectively. After some algebras, we have
\[ \tau_{R \textit{x'}} = \frac{\pi}{2} \int d\varepsilon [f(\varepsilon) - f(\varepsilon + eV)] (D_{R^\dagger} + D_{R^\dagger}) \Gamma^L_1(P_1 \sin \theta - P_3 \cos \theta), \]
where \( P_1 = \frac{D_{L\uparrow}(T_2^1 - T_2^2) - D_{L\downarrow}(T_2^2 - T_2^3)}{D_{L\uparrow}(T_2^1 + T_2^2) + D_{L\downarrow}(T_2^2 + T_2^3)} \), \( P_3 = \frac{2(D_{L\uparrow}T_3 + D_{L\downarrow}T_4)}{D_{L\uparrow}(T_2^1 + T_2^2) + D_{L\downarrow}(T_2^2 + T_2^3)} \), and \( \Gamma_1^L = D_{L\uparrow}(T_2^2 + T_2^3) + D_{L\downarrow}(T_2^3 + T_2^4) \). It is interesting to note from the above equation that the direction of the spin torque is closely related to whether the applied bias is positive or negative, namely, it depends strongly on the direction of the electrical current, in agreement of the previous observation [2,4–7].

To compare the results with those reported in Refs. [2,9], we can also consider the spin-torque per current, i.e. \( \tau_{Rx}' / I_e = \langle \frac{1}{G} \frac{\partial \tau_{Rx}'}{\partial V} \rangle \), where \( G \) is the tunneling conductance [see Eq. (12) in Ref. [17]] and \( V \) is the applied bias. Then we obtain

\[
\tau_{Rx}' / I_e = \frac{\hbar}{e} \frac{P_1 \sin \theta - P_3 \cos \theta}{1 + P_2(P_1 \cos \theta + P_3 \sin \theta)},
\]

where \( P_2 = \frac{D_{R\uparrow} - D_{R\downarrow}}{D_{R\uparrow} + D_{R\downarrow}} \) is the polarization of the right ferromagnet, and the energy is taken at the Fermi level.

To gain deeper insight into the effect of the spin-flip scatterings on the spin transfer torque, we ought to invoke numerical calculations. Before presenting the calculated results, we shall presume a parabolic dispersion for band electrons based on which the DOS of conduction electrons are calculated. The Fermi energy and the molecular field will be taken as \( E_f = 1.295 \) eV and \( |\mathbf{h}_1| = |\mathbf{h}_2| = 0.90 \) eV, which are given in Ref. [18] for Fe. In addition, we may for convenience introduce two parameters \( \gamma_1 = T_2 / T_1 \) and \( \gamma_2 = T_3 / T_1 \), and assume \( T_1 = T_4 \).

Now let us first look at the case without the spin-flip scatterings. The leading contribution to the torque \( \tau_{Rx}' \) comes from the first nonvanishing term. When the spin-flip scatterings are absent, i.e. \( T_2 = T_3 = 0 \), we find that

\[
\frac{\partial \tau_{Rx}'}{\partial V} = \frac{\xi}{2}(D_{R\uparrow} + D_{R\downarrow})(D_{L\uparrow} + D_{L\downarrow})T_1^2 P_1 \sin \theta
\]

with \( P_1 = (D_{L\uparrow} - D_{L\downarrow})/(D_{L\uparrow} + D_{L\downarrow}) \), which is consistent with that obtained in Refs. [2,3]. This result shows clearly that \( \tau_{Rx}' \) vanishes when the relative alignment of magnetizations of the two ferromagnets is parallel (\( \theta = 0 \)) or antiparallel (\( \theta = \pi \)). It is similar to that for a FM-NM-FM trilayer system discussed in Ref. [9], although the transport mechanisms are different. The present result can be easily understood because the spin-polarized electrons along the \( z \) or \(-z\) axis cannot feel the spin transfer torque owing to the property of
\(\vec{s}_1 \times (\vec{s}_1 \times \vec{s}_2)\). In Fig. 2, we show the \(\theta\) dependence of the spin torque \(\frac{\tau_{Rx'}}{I_e}\) in the absence of spin-flip scatterings for different polarizations. One may see that \(\frac{\tau_{Rx'}}{I_e}\) is a nonmonotonic function of \(\theta\), and shows minima and maxima at certain relative alignments. \(\frac{\tau_{Rx'}}{I_e}\) versus \(\theta\) is inversion-symmetrical to the axis of \(\theta = 0\). It is evident that the larger the polarization, the stronger the spin transfer torques. This observation is in good agreement with the finding in Ref. [2], though the latter is obtained on a basis of a quite different method.

The \(\theta\)-dependence of \(\frac{\tau_{Rx'}}{I_e}\) for \(\gamma_1 = \gamma_2\) is shown in Fig. 3 (a). It can be seen that the spin-flip scatterings can lead to a nonvanishing spin torque at \(\theta = 0\) or \(\pi\), i.e. 
\[
\frac{\partial \tau_{Rx'}}{\partial V} = \mp e\pi (D_{R\uparrow} + D_{R\downarrow})T_1^2(\gamma_1 D_{L\uparrow} + \gamma_2 D_{L\downarrow}),
\]
being different from the case when the spin-flip scatterings are neglected. However, in the present case with \(\gamma_1 = \gamma_2 = 0.05\), at a particular angle, e.g. \(\theta = 14.04^\circ\), \(\tau_{Rx'}\) becomes zero. This suggests that the spin-flip scattering can lead to an angular shift to the spin torque. In other words, the spin-flip scattering gives rise to an additional torque which we may call the spin-flip induced spin torque henceforth. In addition, if \(\gamma_1 = \gamma_2 = \gamma\), one may find that \(\frac{\partial \tau_{Rx'}}{\partial V}\) is proportional to \(\gamma\). When \(\gamma_1 \neq \gamma_2\), which means that the spin-flip scatterings from the spin up band to the spin down band are different from those from down to up, \(\gamma_1\) and \(\gamma_2\) give different effects on the \(\theta\)-dependence of spin torques as shown in Fig. 3 (b). It is observed that there are angular shifts for different \(\gamma_1\) and \(\gamma_2\), showing that the effects of \(\gamma_1\) and \(\gamma_2\) are various. For instance, the curve for \(\gamma_1 = 0.2\) and \(\gamma_2 = 0.1\) moves to the right-hand side in comparison to the curve of \(\gamma_1 = 0.1\) and \(\gamma_2 = 0.2\). It appears that a larger spin-flip scattering from spin down to spin up has a larger effect on the spin torque.

The effect of the molecular fields of the ferromagnets on the spin torques is also investigated. The \(\theta\)-dependences of \(\tau_{Rx'}\) are shown in Fig. 4 for different parameter \(\alpha = |\vec{h}_R|/|\vec{h}_L|\). One may find that \(\tau_{Rx'}/I_e\) is also a nonmonotinic function of \(\theta\), and shows peaks at certain values of \(\theta\) for different \(\alpha\)'s. It is interesting to note that the two crossing points at \(\theta_1 = 37^\circ\) and \(\theta_2 = 127^\circ\) under different molecular fields are observed. When \(\theta < \theta_1\), a larger \(\alpha\) leads to a smaller magnitude of the spin-torque (which are negative); when \(\theta_1 < \theta < \theta_2\), the larger
α, the smaller the spin-torques; while θ > θ_2, a larger α leads to a larger magnitude of the spin-torque, showing that |h_R| and |h_L| have different effects on the spin torques. The two crossing points appeared in the curve τRx'/I_e versus θ for different molecular fields can be understood in the following way. From Eq. (8), one can get a relation
\[ \frac{τ_{Rx'}}{I_e} = \frac{h}{e} \sqrt{P_1^2 + P_3^2} \sin(θ - θ_f), \]
where the angular shift θ_f is defined by \( \tan θ_f = \frac{P_3}{P_1} \) [17]. θ_1 at which the first crossing point appears is nothing but θ_f (i.e. θ_1 = θ_f = 37°). At θ_1 = θ_f, \( \frac{τ_{Rx'}}{I_e} = 0 \), which is independent of the molecular field of the right ferromagnet. The second crossing point appears at \( θ_2 - θ_f = \frac{π}{2} \) (i.e. \( θ_2 = 127° \)). At this angle \( θ_2 \), \( \frac{τ_{Rx'}}{I_e} = \frac{h}{e} \sqrt{P_1^2 + P_3^2} \), which depends only on the parameters of the left ferromagnet but is independent of the molecular field of the right ferromagnet. Therefore, at these two particular alignments, \( \frac{τ_{Rx'}}{I_e} \) gives the same value for different α’s, thereby leading to the two crossing points. When the spin-flip scattering disappears, the two crossing points occur at θ = 0 and \( \frac{π}{2} \). So we may find that the spin-flip scattering may lead to an additional spin torque on the magnetic moments of the right ferromagnet. The present observation may be readily understood, because the spin-flip tunneling of electrons from the left ferromagnet into the right ferromagnet would give rise to a change of the DOS of conduction electrons as well as the effective polarization factor in the right ferromagnet, leading to an additional torque exerting on the magnetic moments, thereby the property of an angular shift of the spin torque was observed.

In summary, we have investigated the current-induced spin torque in FM-I-FM tunnel junctions with inclusion of spin-flip scattering by using the nonequilibrium Green function method. In the absence of the spin-flip scattering, our results are consistent with the previous results found in Refs. [2,3,9]. When the spin-flip scattering, the factor that could exist in realistic spin-based electronic devices, is considered, we have found that an additional spin torque is induced. It is found that the spin-flip scattering can enhance the maximum of the current-induced spin transfer torque, giving rise to an angular shift. The effects of the molecular fields of the left and right ferromagnets on the spin torques are also studied.

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It can be observed that the spin-torques per unit tunneling current exerting on the right ferromagnet are independent of the molecular field of the right ferromagnetic lead at $\theta = \theta_f$ and $\theta - \theta_f = \frac{\pi}{2}$. The present study shows that the spin-flip scatterings during the tunneling process in magnetic tunnel junctions have indeed remarkable influences on the dynamics of the magnetic moments. Since the spin-transfer torque induced by the applied current can switch the magnetic domains between different orientations [6], people can invoke this property to fabricate a current-controlled magnetic memory element. As the previous studies on the spin torque usually ignore the effect of the spin-flip scatterings which could not be avoided in practice, our investigation might offer a supplement to the previous studies, namely, when people design a device based on a mechanism of the spin transfer torque, one should take the additional torque induced by the spin-flip scatterings into account, which could complement with the experiments.

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FIGURE CAPTIONS

Fig. 1 A schematic illustration of the spin-transfer torque with spin-flip scatterings in a $FIF$ tunnel junction.

Fig. 2 Spin transfer torque $\frac{\tau_{Rx}'}{I_e}$ versus angle $\theta$ in the absence of the spin-flip scatterings (i.e. $\gamma_1 = \gamma_2 = 0$). Equal polarization factors of the magnets are assumed ($P_1 = P_2$). Torque per unit current is measured in unit of $\hbar/e$.

Fig. 3 The $\theta$ dependence of $\frac{\tau_{Rx}'}{I_e}$ for (a) $\gamma_1 = \gamma_2$ and (b) $\gamma_1 \neq \gamma_2$, where the effective masses of the left and right ferromagnets are taken as unity, the molecular fields are assumed to be 0.9 eV, the Fermi energy is taken as 1.295 eV, and $T_1 = T_4 = 0.01$ eV. Torque per unit current is measured in unit of $\hbar/e$.

Fig. 4 $\frac{\tau_{Rx}'}{I_e}$ versus angle $\theta$ for different molecular fields. Here we take $\gamma_1 = \gamma_2 = 0.15$, $|h_1| = 0.9$ eV, and the other parameters are taken the same as those in Fig. 3. Torque per unit current is measured in unit of $\hbar/e$. 

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Electrons flow along the x-axis

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Fig. 2 Zhu et al
Fig. 3 Zhu et al
Fig. 4 Zhu et al

\[ \frac{\tau_{Rx}'}{I_c} \]

- \( \alpha = 0.5 \)
- \( \alpha = 0.8 \)
- \( \alpha = 1 \)
- \( \alpha = 1.3 \)