Electric and thermal spin transfer torques across ferromagnetic/normal/ferromagnetic graphene junctions

Zhi Ping Niu and Meng Meng Wu

College of Science, Nanjing University of Aeronautics and Astronautics, Jiangsu 210016, People's Republic of China

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Abstract

We investigate the spin transfer torque (STT) driven by electric bias voltages across and temperature gradients through ferromagnetic/normal/ferromagnetic graphene junctions. Due to the unique band structure of the ferromagnetic graphene, there exists two transport regimes: the electron to electron (I) and hole to electron (II) transport. The electric STTs originated from the two regimes have opposite sign and can be reduced by the competition between the two transport processes. On the contrary, the thermal STTs originated from the transport regimes I and II have the same sign and are enhanced when the two regimes coexist. Remarkably, the thermal STT is comparable with the electric STT. Furthermore, the electric and thermal counterpart can be manipulated by the Fermi level. The controllable STT reported here makes the ferromagnetic graphene junction ideal for future spintronics applications.

1. Introduction

Spin transfer torque (STT) in tunnel junctions with ferromagnetic electrodes is one of the essential underlying phenomena of spintronics [1, 2]. The magnetization direction of a ferromagnetic thin layer can be reoriented by the transfer of angular momentum from a spin polarized current. The STT, which provides an ultralow-power switching (writing) solution, is predicted to be the next key step toward the development of high-density non-volatile magnetic random access memories devices [3–7]. For radio frequency devices, a new type of an integrated STT nanooscillator has been proposed for telecommunication [7, 8]. Moreover, the STT also has the potential application in domain wall motion [9], magnetic sensors [10] and spin torque diode [11]. Therefore, the STT has attracted much attention [2–17] since it first predicted independently by Slonczewski and Berger [1]. Recently, the STTs in two-dimensional materials such as phosphorene [18], topological insulator [19, 20] and graphene [21–25] have also been reported. Due to the coupling between the valley and spin degrees of freedom, Niu [25] predicted a valley controlled STT in normal/normal/ferromagnetic graphene junctions. Although the STT in ferromagnetic graphene junctions has been discussed in references [21–25], the authors only focused on the zero bias limit, and the effect of the bias voltage on the STT is not clear.

On the other hand, in magnetic materials spin polarized currents can be created by thermal currents [26–31]. The transfer of spin angular momentum through this process has been named thermal STT [26, 27]. The thermal STT in metallic spin valves was theoretically predicted [27] and then experimentally observed [28]. The thermal STT in MgO based magnetic tunnel junctions has also been extensively explored [26, 32–34]. In order to be sufficient to switch the magnetic configurations, very thin barriers of 3 MgO atomic layers are needed [26, 33, 34]. Heiliger et al [34] pointed out that even for such a thin barrier the thermal STT is still too small for reorienting the magnetic order and further optimization is needed. Thus it is highly challenging to induce magnetic tunnel junction switching by virtue of the thermal STT. Unlike the MgO based magnetic tunnel junctions, in graphene junctions the Klein tunneling process appears, and the exponential decay of the current with barrier thickness is absent. Therefore, it is expected...
that a large thermal STT can be observed in magnetic graphene junction. However, the thermal STT in magnetic graphene junctions has not been explored.

In this work, the electric and thermal STTs through ferromagnetic/normal/ferromagnetic ($F_1/N/F_2$) graphene junctions are studied. We compare the electric STT with the thermal STT. Due to the unique band structure of the ferromagnetic graphene, there exists two transport regimes: the electron to electron and hole to electron transport. The coexistence of the two regimes can reduce the electric STT but enhance the thermal STT. Remarkably, the thermal STT is comparable with the electric STT. Furthermore, the STT can be manipulated by the Fermi level.

2. Model and formulation

We consider a two-dimensional $F_1/N/F_2$ graphene junction under the electric bias $V_b$ or the temperature gradient $\Delta T$, as shown in figure 1. Here the temperature gradient is defined as $\Delta T = T_L - T_R$, where $T_L$ ($T_R$) is the temperature in the left (right) lead. The interfaces between the ferromagnetic/normal regions locate at $x = 0$ and $x = L$ with the normal region width $L$. In the $F_1$, a graphene monolayer sheet in the $xy$ plane is grown on a substrate such as SiC that provides a staggered potential $(\lambda_v)$ sites. We assume that $F_1$ is ferromagnetic, while that of the $F_2$ is along the $z$ axis, and that of the $F_2$ is along the $\alpha$ axis by an angle $\alpha$. $\tau_{z\alpha}$ is along $x'$ direction in the $x'y'z'$ coordinate frame.

2.1 Hamiltonian

The Hamiltonian of the present junction is expressed as

$$
H(k_y) = -\tau \sum_{m,\sigma} \left[ c_{m, k_y, \sigma}^\dagger c_{m+1, k_y, \sigma} e^{-ik_ya/2} + c_{m, k_y, \sigma}^\dagger c_{m-1, k_y, \sigma} e^{ik_ya/2} + c_{m, k_y, \sigma}^\dagger c_{m, k_y, \sigma} e^{ik_ya} + c.c. \right]
$$

$$
+ \tau \sum_{m,\sigma,\sigma'} (\varepsilon_m - \sigma \cdot \mathbf{M} + \mu_m \lambda_v) c_{m, k_y, \sigma}^\dagger c_{m, k_y, \sigma'}
$$

(1)

Here $c_{m, k_y, \sigma}^\dagger$ ($c_{m, k_y, \sigma}$) with $\beta = A, B$ and $\sigma$ $(\sigma') = \uparrow, \downarrow$ stands for the creation (annihilation) operator of an electron with spin $\sigma$ at site $m$. $\varepsilon_m$ is the on-site energy, which is set as $\varepsilon_0$ in the $F_2$ and zero in the $F_1$. Under the applied bias $V_b$ the potential inside the normal region $\varepsilon_m = -eV_b \frac{m}{N-1}$ varies linearly with $m$ [13, 14], where the normal region width is $L = \sqrt{3}Na/2$ with $a$ the carbon–carbon distance in graphene. $\mathbf{M}$ represents the exchange field and we assume $\mathbf{M} = \mathbf{M}_L$ and $\mathbf{M} = \mathbf{M}_R$ in the $F_1$ and $F_2$, respectively. The magnetization direction of the $F_1$ is along $z$ axis, while that of the $F_2$ is along $(\sin \alpha, 0, \cos \alpha)$. The last term is the staggered potential with $\lambda_v$ induced by the graphene-substrate interaction, where $\mu_m$ is 1 ($-1$) for $A$ ($B$) sites. We assume that $\lambda_v$ is only finite in the $F_1$.

The STT is studied by the non-equilibrium Green’s function method. The retarded Green’s function $G'$ is calculated by using the iteration technique developed by Lopez-Sancho et al [37]. The in-plane STT $\tau_{x'}$ acting on the $F_2$ can be obtained as [23–25]

$$
\tau_{x'} = \frac{1}{2\pi} \int \tau_{x'}(E) \left( f_L - f_R \right) dE.
$$

(2)

Here $\tau_{x'} \propto \mathbf{M}_R \times (\mathbf{M}_R \times \mathbf{M}_L)$ [9] is along the $x'$ direction in the $x'y'z'$ coordinate frame (figure 1). The energy $E$ dependent in-plane torque $\tau_{x'}(E)$ is expressed as $\tau_{x'}(E) = \sum_{k_y} \text{Tr}$
two transport regimes I and II, as shown in figure 2(b). Depending on τ increases, the angular dependence of the electric STT for the left and right leads, respectively. In this work like the previous works \[23–25\] we on ot c e n s i d e r t h e simplicity, we set its effect.

vanishing τ with E comes from the electron to electron transport (regime I marked in figure 2(b)). With increasing \(|V_b|\), the spin polarized currents acting on the F2 increases, so τ\(_{\alpha}\) monotonically increases with \(|V_b|\). On the other hand, for the positive bias \(\tau_{\alpha}\) exhibits a nonmonotonic bias dependence. \(\tau_{\alpha}\) first increases and then decreases with \(V_b\). When \(V_b\) is further enhanced, \(\tau_{\alpha}\) reverses its sign and increases monotonically. We can

\[
\frac{\Gamma_L G^+ \Gamma_R (\sigma_x \cos \alpha - \sigma_z \sin \alpha)}{\Gamma_L (\Gamma_R)} \] 

with \(\Gamma_L (\Gamma_R)\) the line-width function of the left (right) lead.

\[
f_{(R)} = \frac{1}{1 + \exp \left[ (E - E_F + eV_{(R)})/k_B T_{(R)} \right]} \] 

with the Fermi level \(E_F\) stands for the Fermi distribution function in the L (R) lead. For the STT driven by the electric bias, the bias voltages are \(V_L = 0\) and \(V_R = V_b\) for the left and right leads, respectively. In this work like the previous works \[23–25\] we do not consider the out-plane torque \(\tau_y\). This is because \(\tau_y\) show a similar feature but its magnitude is very small, so we neglect its effect.

3. Electric spin-transfer torque

The angular dependence of the electric STT \(\tau_{\alpha}\) at various Fermi levels is investigated in figure 2. For simplicity, we set \(t = 1\) and \(e = 1\). In the numerical calculations, the parameters \(\lambda_\alpha = \hbar = 0.005\), \(\epsilon_0 = -0.2\), and \(N = 4\) are taken. \(\tau_{\alpha}\) is in units of \(eV\) throughout this work. The curves of \(\tau_{\alpha}\) versus \(\alpha\) essentially follow the usual sinusoidal behavior. For the parameters taken here, when \(E_F\) increases, \(\tau_{\alpha}\) first decreases, then reverses its sign and increases successively. This can be understood by the two transport regimes I and II, as shown in figure 2(b). Depending on \(E_F\) and \(V_b\) the transport is divided into electron-to-electron I and hole-to-electron II regimes, where the incident currents from the F1 are initially spin polarized along \(z\) and \(-z\) directions, respectively. Thus the STTs originated from the two regimes have the opposite sign and can cancel each other out, leading to the nonmonotonic behavior of \(\tau_{\alpha}\).

We also confirm this by analyzing the energy dependent torque \(\tau_{\alpha}(E)\), as shown in the inset of figure 3. For zero \(E_F\) \(\tau_{\alpha}\) only arises from the hole to electron transport. When \(E_F\) is finite, for \(E_F < V_b\) the electron-to-electron transport also contributes to \(\tau_{\alpha}\). Thus \(\tau_{\alpha}\) decreases due to the competition between the transport processes in the I and II regimes. For example, \(\tau_{\alpha}(E)\) at \(V_b = 2E_F\) is plotted in the inset of figure 3. In this case the transport window is \(|E| < E_F\). The energy dependent torques in the I (0 < \(E < E_F\)) and II (\(-E_F < E < 0\)) regimes have the opposite sign, but the difference of the Fermi distribution functions \(f_L - f_R\) is an even function of \(E\), so \(\tau_{\alpha}\) from the two regimes almost cancels each other out, leading to a vanishing \(\tau_{\alpha}\). On the other hand, when \(E_F\) exceeds \(V_b\), \(\tau_{\alpha}\) only comes from the I regime and varies slightly with \(E_F\).

We display the bias \(V_b\) dependence of \(\tau_{\alpha}\) at various \(\alpha\) in figure 3. For the negative \(V_b\), the current only comes from the electron to electron transport (regime I marked in figure 2(b)). With increasing \(|V_b|\), the spin polarized currents acting on the F2 increases, so \(\tau_{\alpha}\) monotonically increases with \(|V_b|\). On the other hand, for the positive bias \(\tau_{\alpha}\) exhibits a nonmonotonic bias dependence. \(\tau_{\alpha}\) first increases and then decreases with \(V_b\). When \(V_b\) is further enhanced, \(\tau_{\alpha}\) reverses its sign and increases monotonically. We can

Figure 2. (a) \(\tau_{\alpha}\) as a function of \(\alpha\) at various \(E_F\) with the parameters of \(V_b = 0.002\) and \(T = \Delta T = 0\,\text{K}\). Along the arrow, \(E_F/V_b = 0, 0.5, 1.0, 1.5,\) and 2.0. (b) The band structures in the F1 (left) and F2 (right) regions. Here the black (red) lines correspond to the spin up (spin down) subband.

\[
\frac{\Gamma_L G^+ \Gamma_R}{\Gamma_L (\Gamma_R)} \] 

with \(\Gamma_L (\Gamma_R)\) the line-width function of the left (right) lead.

\[
f_{(R)} = \frac{1}{1 + \exp \left[ (E - E_F + eV_{(R)})/k_B T_{(R)} \right]} \] 

with the Fermi level \(E_F\) stands for the Fermi distribution function in the L (R) lead. For the STT driven by the electric bias, the bias voltages are \(V_L = 0\) and \(V_R = V_b\) for the left and right leads, respectively. In this work like the previous works \[23–25\] we do not consider the out-plane torque \(\tau_y\). This is because \(\tau_y\) show a similar feature but its magnitude is very small, so we neglect its effect.

3. Electric spin-transfer torque

The angular dependence of the electric STT \(\tau_{\alpha}\) at various Fermi levels is investigated in figure 2. For simplicity, we set \(t = 1\) and \(e = 1\). In the numerical calculations, the parameters \(\lambda_\alpha = \hbar = 0.005\), \(\epsilon_0 = -0.2\), and \(N = 4\) are taken. \(\tau_{\alpha}\) is in units of \(eV\) throughout this work. The curves of \(\tau_{\alpha}\) versus \(\alpha\) essentially follow the usual sinusoidal behavior. For the parameters taken here, when \(E_F\) increases, \(\tau_{\alpha}\) first decreases, then reverses its sign and increases successively. This can be understood by the two transport regimes I and II, as shown in figure 2(b). Depending on \(E_F\) and \(V_b\) the transport is divided into electron-to-electron I and hole-to-electron II regimes, where the incident currents from the F1 are initially spin polarized along \(z\) and \(-z\) directions, respectively. Thus the STTs originated from the two regimes have the opposite sign and can cancel each other out, leading to the nonmonotonic behavior of \(\tau_{\alpha}\).

We also confirm this by analyzing the energy dependent torque \(\tau_{\alpha}(E)\), as shown in the inset of figure 3. For zero \(E_F\) \(\tau_{\alpha}\) only arises from the hole to electron transport. When \(E_F\) is finite, for \(E_F < V_b\) the electron-to-electron transport also contributes to \(\tau_{\alpha}\). Thus \(\tau_{\alpha}\) decreases due to the competition between the transport processes in the I and II regimes. For example, \(\tau_{\alpha}(E)\) at \(V_b = 2E_F\) is plotted in the inset of figure 3. In this case the transport window is \(|E| < E_F\). The energy dependent torques in the I (0 < \(E < E_F\)) and II (\(-E_F < E < 0\)) regimes have the opposite sign, but the difference of the Fermi distribution functions \(f_L - f_R\) is an even function of \(E\), so \(\tau_{\alpha}\) from the two regimes almost cancels each other out, leading to a vanishing \(\tau_{\alpha}\). On the other hand, when \(E_F\) exceeds \(V_b\), \(\tau_{\alpha}\) only comes from the I regime and varies slightly with \(E_F\).

We display the bias \(V_b\) dependence of \(\tau_{\alpha}\) at various \(\alpha\) in figure 3. For the negative \(V_b\), the current only comes from the electron to electron transport (regime I marked in figure 2(b)). With increasing \(|V_b|\), the spin polarized currents acting on the F2 increases, so \(\tau_{\alpha}\) monotonically increases with \(|V_b|\). On the other hand, for the positive bias \(\tau_{\alpha}\) exhibits a nonmonotonic bias dependence. \(\tau_{\alpha}\) first increases and then decreases with \(V_b\). When \(V_b\) is further enhanced, \(\tau_{\alpha}\) reverses its sign and increases monotonically. We can
explain this nonmonotonic behavior by analyzing the two transport processes indicated in figure 2(b). For \( V_b < E_F \) with increasing \( V_b \) the spin polarized current from the I regime acting on the F2 increases, resulting in the enhancement of \( \tau_x' \). When \( V_b \) exceeds \( E_F \), the hole-to-electron transport also appears, so because of the competition between the transport processes in the I and II regimes \( \tau_x' \) decreases with \( V_b \). When \( V_b \) is further enhanced, \( \tau_x' \) is determined by the II regime and increases.

### 4. Thermal spin-transfer torque

Next, the thermal STT \( \tau_x' \) as a function of \( \alpha \) at various Fermi levels is shown in figure 4. Here the current is only driven by the temperature gradient. Similar to the electric STT, the angular dependence of the thermal STT is a sine dependence. The amplitude of \( \tau_x' \) decreases with \( E_F \). For large \( E_F \), \( \tau_x' \) becomes very small and even reverses its sign. The behavior of \( \tau_x' \) can be illustrated from the following fact. At zero \( E_F \) the spin up current from the electron to electron transport and the spin down one from the hole to electron transport counterpropagate, so the thermal STTs from the regimes I and II marked in figure 2(b) have the same sign, and can be enhanced when the two regimes are involved. This is different from \( \tau_x' \) driven by \( V_b \), where the electric STTs from the two regimes have the opposite sign and are reduced by the competition between the two transport processes. We also confirm this feature by studying \( \tau_x'(E) \) and \( f_L - f_R \), as shown in the inset of figure 4. \( \tau_x'(E) \) and \( f_L - f_R \) in the I (\( E > 0 \)) and II (\( E < 0 \)) regimes have the opposite sign, so \( \tau_x'(E)(f_L - f_R) \) has the same sign in the regimes I and II and the coexistence of the two transport processes can enhance \( \tau_x' \). When \( E_F \) is finite, for \( E > 0 \) \( \tau_x'(E) \) has the same sign for each energy, but \( f_L - f_R \) antisymmetric with respect to \( E_F \), so part of \( \tau_x' \) from the electron current cancels that from the hole current, leading to the
Figure 5. (a) $\tau_x'$ versus $\Delta T$ at different $\alpha$. (b) $\tau_x'$ at $V_b = 0$ (solid line), $V_b = 0.002$ (dashed line), and $V_b = 0.004$ (dotted line) versus $\Delta T$. In the inset of figure 5(b) we plot $f_L - f_R$ versus $E$.

decrease of $\tau_x$. For large $E_F$, $\tau_x'$ from the electron and hole currents almost cancels each other out, leading to a small $\tau_x'$.

In figure 5(a) $\tau_x'$ versus $\Delta T$ at $k_B T = 0.001$ and various $\alpha$ is plotted. Because at zero $E_F$ the incident current is enhanced by $\Delta T$, $\tau_x$ increases monotonically with $\Delta T$. At fixed $\Delta T$ when $\alpha$ sweeps from zero to $\pi/2$, $\tau_x'$ increases with $\alpha$, which is consistent with figure 4. In particular, it is worthy noted that the thermal STT is comparable with the electric STT. In addition, we also study $\tau_x'$ versus $\Delta T$ at large $E_F$ (not shown), where the features of the STT are quite similar to these in figure 5(a), except that the magnitude of the STT is very small. In the discussion above we focus on comparing the electric STT with the thermal STT, so we do not consider the bias voltages and temperature gradients simultaneously. If both the bias voltages and temperature gradients are considered, the electric STT and thermal STT occur at the same time. In figure 5(b) we study $\tau_x'$ versus $\Delta T$ at various $V_b$. With the increase of $\Delta T$, due to the competition between the electric STT and its thermal counterpart the STT first decreases. When $\Delta T$ is further enhanced, the thermal STT begins to play a dominant role, so the STT increases monotonically with $\Delta T$. We can also confirm the feature of the STT by analyzing $\tau_x(E)$ and $f_L - f_R$. $\tau_x(E)$ is almost antisymmetrical about $E = 0$ (see the inset of figure 3). As shown in the inset of figure 5(b) in the presence of $V_b f_L - f_R$ is redistributed and shifts to negative $E$ and the antisymmetry about $E = 0$ does not hold, so $\tau_x'(f_L - f_R)$ is redistributed and its energy integration $\tau_x'$ depends on $V_b$ and $\Delta T$.

5. Summary

In summary, we have theoretically investigated the electric and thermal STT across $F_1/N/F_2$ graphene junctions. We compare the electric STT with the thermal STT. It is found that there exists two transport regimes I and II, where the currents originate from the electron to electron (I) and hole to electron (II) transport, respectively. The electric STTs originated from the two regimes have opposite sign and are reduced when both regimes are involved, which leads to a nonmonotonic bias dependence. However, the thermal STTs originated from the two regimes have the same sign and are enhanced by the coexistence of
both regimes. Remarkably, the thermal STT is comparable with the electric STT. Furthermore, the electric and thermal STT can be manipulated by the Fermi level. The controllable STT obtained here suggests the ferromagnetic graphene junction ideal for future spintronics applications.

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ORCID iDs

Zhi Ping Niu https://orcid.org/0000-0003-3943-4335

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