First-principles study of spin-transfer torque in Co$_2$MnSi/Al/Co$_2$MnSi spin-valve

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The spin-transfer torque (STT) effect$^\text{[1, 2]}$ has attracted considerable interest in the recent years due to its potential applications on future spintronics devices, such as the STT-based magnetic random access memory (STT-MRAM)$^\text{[3, 4]}$ and spin-transfer nanocontact oscillator (STNO)$^\text{[5, 6]}$. However, in STT-MRAM the biggest challenge is to reduce the switching current density that mainly depends on the efficiency of current-induced STT, i.e. the STT per current. Writing information by STT in MRAM with low switching current can save power consumption and shrink the size of memory cell, which are of crucial importance to realistic applications. Another important issue is the angular dependence of STT in STNO devices, where the asymmetry parameter $\Lambda$ dominates the output power of high-frequency generation.$^\text{[7, 8]}$

In order to reduce the critical current, the Co-based Heusler alloys, such as Co$_2$MnSi (CMS) and Co$_2$FeAl (CFA) etc., are believed as good candidates for STT-based memory devices.$^\text{[9]}$ These Heusler compounds not only have small damping constant, low saturation magnetization$^\text{[10, 11]}$ and perpendicular magnetic anisotropy,$^\text{[12–14]}$ but also have been theoretically predicted to be half-metallic materials with very high spin polarization (P$\approx 1$).$^\text{[15]}$ which are all in favour of decreasing critical current.$^\text{[1, 2]}$ Compared to the early all-metallic spin-valve (SV) of conventional ferromagnet such as Co/Cu multilayers system,$^\text{[16–18]}$ the magnetoresistance (MR) ratio and the efficiency of STT will be enhanced for devices fabricated by half-metallic Heusler alloys due to the high spin polarization. On the other hand, the magnetic tunnel junction (MTJ) with Heusler electrodes also shows very large tunneling MR ratio even at room temperature.$^\text{[19–21]}$ However, the main disadvantage of MTJ devices is the large resistance-area product (RA) due to the insulator spacer. So the read-write speed of memory will be reduced for its large RC constant. Meanwhile, the RA of all-metallic structure is apparently much smaller, suggesting that the all-metallic SV of half-metallic Heusler alloys has greater potential for spintronics applications.

Recently, the half-metallic SV system composed of CMS has received increasing attention$^\text{[22–24]}$ because the Curie temperature of CMS is very high (985K) and the lattice of CMS can be well matched with several non-magnetic metals. The perpendicular magnetic anisotropy of CMS also has been reported in CoPt/CMS hybrid electrode,$^\text{[26]}$ which implies that it is suitable for application on high-frequency generation.$^\text{[27–29]}$ So far, for CMS/Al/CMS trilayers there have been investigations that focus on the conductance and its relationship with the interface architectures.$^\text{[29–32]}$ But all these studies do not include the transport properties for disorder interface and the first-principles calculation of STT in CMS/Al/CMS SV system has not been reported up to now. Further, the dependence of STT on CMS/Al interface architectures is still unclear yet. Therefore, the main purpose of this paper is to study the magnitude and the angle-dependence of STT in CMS/Al/CMS SV system by first-principles method. In addition, the calculations will be carried out in different CMS/Al interfaces, i.e. Co-terminated (CoCo/Al) and MnSi-terminated (MnSi/Al) interface including alloyed interfacial disorder.

**I. INTRODUCTION**

The spin-transfer torque (STT) effect$^\text{[1, 2]}$ has attracted considerable interest in the recent years due to its potential applications on future spintronics devices, such as the STT-based magnetic random access memory (STT-MRAM)$^\text{[3, 4]}$ and spin-transfer nanocontact oscillator (STNO)$^\text{[5, 6]}$. However, in STT-MRAM the biggest challenge is to reduce the switching current density that mainly depends on the efficiency of current-induced STT, i.e. the STT per current. Writing information by STT in MRAM with low switching current can save power consumption and shrink the size of memory cell, which are of crucial importance to realistic applications. Another important issue is the angular dependence of STT in STNO devices, where the asymmetry parameter $\Lambda$ dominates the output power of high-frequency generation.$^\text{[7, 8]}$

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Recently, the half-metallic SV system composed of CMS has received increasing attention$^\text{[22–24]}$ because the Curie temperature of CMS is very high (985K) and the lattice of CMS can be well matched with several non-magnetic metals. The perpendicular magnetic anisotropy of CMS also has been reported in CoPt/CMS hybrid electrode,$^\text{[26]}$ which implies that it is suitable for application on high-frequency generation.$^\text{[27–29]}$ So far, for CMS/Al/CMS trilayers there have been investigations that focus on the conductance and its relationship with the interface architectures.$^\text{[29–32]}$ But all these studies do not include the transport properties for disorder interface and the first-principles calculation of STT in CMS/Al/CMS SV system has not been reported up to now. Further, the dependence of STT on CMS/Al interface architectures is still unclear yet. Therefore, the main purpose of this paper is to study the magnitude and the angle-dependence of STT in CMS/Al/CMS SV system by first-principles method. In addition, the calculations will be carried out in different CMS/Al interfaces, i.e. Co-terminated (CoCo/Al) and MnSi-terminated (MnSi/Al) interface including alloyed interfacial disorder.

**II. COMPUTATIONAL METHOD**

In this paper, we employ the tight-binding linearized muffin-tin-orbital (TB-LMTO) surface Green function method with atomic sphere approximation (ASA) to obtain the effective single-electron potential of CMS/Al(001) interface.$^\text{[33–35]}$ The coherent potential approximation (CPA)$^\text{[31, 32]}$ is introduced to deal with the alloyed interfacial disorder. With the rigid potential approximation,$^\text{[33]}$ the effective potential for atomic
spheres in fixed magnet of SV is rotated an angle \( \theta \) relative to the free magnet in spin space. So the STT can be calculated by the corresponding noncollinear scattering wave-function with TB-LMTO basis.\textsuperscript{33,36}

In our calculation the CMS/Al/CMS/Al(001) SV system is composed of a fixed semi-infinite CMS as left lead, a spacer layer with 9 Al monolayers (MLs), a free ferromagnetic layer with 13 CMS MLs and a semi-infinite Al as right lead. Here the three CMS/Al interfaces are assumed to be the same architectures. The magnetization of free CMS layer is align with \( z \) axis. The direction of magnetization for left fixed CMS lead is rotated at a relative angle \( \theta \) in \( x-z \) plane (in-plane). So the transport direction is along the \( y \) axis (out-of-plane). The other details of interface model and electronic structure calculations can be found in our previously work.\textsuperscript{37} For evaluating the STT with clean interface, we use 960 \( \times \) 960 \( k \)-points in full two-dimensional (2D) Brillouin zone (BZ) to obtain the convergent results. However, considering the computational cost, the out-of-plane STT in the case of disorder interface is not included in this work. In addition, for disorder interface the convergence of in-plane STT can be obtained by a \( k_{||} \) sampling equivalent to 50 \( \times \) 50 \( k \)-points in 2D BZ.

### III. RESULTS AND DISCUSSION

First, Fig.1 shows the calculated angular dependence of the total STT on local spins in free CMS layer and the total conductance in CMS/Al/CMS/Al SV system with clean CoCo/Al and MnSi/Al interface. One can see that the in-plane STT deviates from the sine function and the peak of in-plane STT is around \( \theta = 155^\circ \) for CoCo/Al and \( \theta = 140^\circ \) for MnSi/Al. According to Slonczewski model,\textsuperscript{7} these angular-dependent STT can be fitted to the asymmetry parameter of \( \Lambda \approx 4.5 \) for CoCo/Al and \( \Lambda \approx 2.9 \) for MnSi/Al. These values are much larger than that of SV with conventional ferromagnet such as Co/Ni multilayers system (\( \Lambda \approx 1.5 \)),\textsuperscript{28} which can be attributed to the high spin polarization (P=1) originating from the half-metallic nature of the CMS. Moreover, our calculated results also suggest that the STNO device with clean CoCo/Al interface will have much more output power of high-frequency microwave compared to MnSi/Al.

The situation of out-of-plane STT for two kinds of interface is more complicated. The out-of-plane STT of MnSi/Al has a peak at \( \theta = 160^\circ \) and its magnitude is comparable with the in-plane STT, which may have interesting consequences for the switching process of the SV system. However, the out-of-plane STT of CoCo/Al has no such peak structure as MnSi/Al and there are two sign changes around \( \theta = 70^\circ \) and \( 140^\circ \), which is very similar to the results of Co/Cu/Co spin-valves.\textsuperscript{32,33}

From Fig.1a, one can observe that the maximum of total in-plane STT for MnSi/Al is about twice as large as that for CoCo/Al. Note that our calculated torque is generated by a small bias \( V_b \) in the linear response regime.\textsuperscript{23} Therefore, the STT value shown in Fig.1a denotes the zero bias torque that is defined as variation of the torque with the voltage around zero bias. So for voltage biased applications of SV system, Fig.1a demonstrates the in-plane torque for clean MnSi/Al is much larger than that for clean CoCo/Al.

Similarly, Fig.1b shows the obtained total conductance at \( \theta = 0^\circ \) of MnSi/Al is also larger than that of CoCo/Al, which is consistent with the previous first-principles calculations.\textsuperscript{28,30} Miura \textit{et al.} have pointed out\textsuperscript{21} that this conductance difference is due to the larger 3d component of LDOS at Fermi level for interfacial Co atoms of CoCo/Al compared to that of interfacial Mn atoms of MnSi/Al. Then the conduction electron will get stronger reflection in CoCo/Al interface because the 3d-orbital can be regard as scatters of electron. Indeed,
as shown in the inset of Fig. 1(b), this fact is confirmed by our calculated results, which also agrees with Yu et al.’s calculation in CMS/Al interface. In particular, the ratio of conductance between MnSi/Al and CoCo/Al at $\theta = 0^\circ$ is about 2.4, which is very close to the ratio of maximum STT. Just as expected, our calculations results show that the magnitude of STT is dependent on interface transparency. Clearly, this dependence originates from the fact that the larger electronic current will carry the more spin moments to be absorbed by the local spins.

To reveal the interface transparency and STT in more detail, the $k_x$ dependence of transmittance and the total in-plane STT on free CMS layer for clean CoCo/Al and MnSi/Al interface with $\theta = 150^\circ$ are shown in Fig. 2. Here the transmittance of each $k_x$ point includes spin-flip probability. For both CoCo/Al and MnSi/Al interface the transmittance and the total in-plane STT distribute around the region of projected Fermi surface of CMS and Al. As expected, the distribution of transmittance and the total in-plane STT in 2D BZ is very similar to each other, which indicates that the interface transparency dominates the magnitude of in-plane STT in CMS/Al/CMS/Al SV system. In addition, from Fig. 2 one can observe that the states around $\Gamma$ point are really important to the transport properties as discussions in previous works especially in MnSi/Al interface.

In realistic SV devices it is highly possible that the disorder will exist at the interface. So in order to investigate the effect of interfacial disorder on STT, we employ the model of substitutional disorder alloy interface as in Ref. 34. The details for the model of disorder CMS/Al interface can also be found in Ref. 37. Due to the randomness of disorder configuration, first we have tested the uncertainties of total conductance and total in-plane STT using five CMS($\theta = 90^\circ$)/Al/CMS/Al structures with randomly generated disorder interface. Here the configurations of three CMS/Al interfaces are also different. As shown in the Fig. 3 the maximum spread is about 7% for both conductance and STT, which is close to the case of Co/Cu/Co system and have not substantially influence on the results about concentration dependence.

Fig. 4(a) and (b) show the angular dependence of total in-plane STT on free CMS layer of SV system with different interfacial alloy concentration $x$. It can be see that the shape of the angular dependence of STT becomes more symmetric with increasing concentration $x$, which suggests that the output power of microwave in CMS/Al system will be reduced by interfacial disorder. Here the estimated parameter $\Lambda$ for different $x$ is shown in the inset of Fig. 4(a). For CoCo/Al interface $\Lambda$ decreases rapidly as increasing concentration $x$, while for MnSi/Al the influence of interfacial disorder on asymmetry parameters is relatively small. However, even for interfacial disorder at concentration $x = 0.5$, the values of asymmetry parameters for both interface are still relatively large ($\Lambda \approx 2.2$ for CoCo/Al and $\Lambda \approx 2.6$ for MnSi/Al) compared to the case of conventional ferromagnet. Therefore, our results indicate that the CMS/Al/CMS/Al SV system might be a good candidate for STNO applications.

From Fig. 4(b) and (d), one can observe that the maximum of STT and total conductance of parallel configuration for MnSi/Al decrease monotonically with increasing $x$, except the in-plane STT for $x = 0.1$ is approximately equal to that for the clean interface. However, contrary to the case of MnSi/Al, Fig. 4(a) shows for CoCo/Al interface the maximum of STT will increase slightly once the interfacial disorder has been introduced. Then for $x = 0.5$ it will decrease to the same value as that of clean interface. Meanwhile, Fig. 4(c) shows the total conductance of parallel configuration for CoCo/Al is significantly enhanced by the interfacial disorder. A similar phenomenon is also observed in Fe/Cr interface, where the conductance can be enhanced by a factor of three.
to the electronic structure mismatch between the CMS and Al layer. As the above discussion of clean interface, the larger $3d$ LDOS of interfacial Co atoms of CoCo/Al is responsible for the higher reflection of propagating electrons. With the mixture of Al atoms in the interfacial region, the reflection of incoming electron will be reduced due to the $3d$ orbital of Al atoms is empty. Interestingly, despite the SV with clean MnSi/Al will obtain larger torque and conductance compared to clean CoCo/Al, our calculated results show that when the degree of interfacial disorder is sufficiently large, these two interfaces will have approximately the same magnitude of torque and conductance.

For the current-induced switching of magnetization in SV system, it is believed that the torque per current is more important parameter. Note that the above calculated result of STT is just in-plane torque $T_{in}(\theta)$ per lateral unit cell. Considering that the area of cross section is $A$, the torque per current can be written as $T_{in}(\theta)/[A \times G(\theta)]$, where $G(\theta)$ is the total conductance. So the parameter $g(\theta)$ for describing STT efficiency can be defined as $g(\theta) = T_{in}(\theta)/[A \times G(\theta)]/\sin \theta$, where $A \times G(\theta)$ is electronic current $I$ that flows through one lateral unit cell at unit bias. This well-known parameter $g(\theta)$ is just the deviation between the curve of angular dependence of STT per current and the sine function, which represents the efficiency of STT for switching the magnetic layer in spin-valve.

Here the calculated $g(\theta)$ for CoCo/Al and MnSi/Al interface are shown in Fig. As a comparison, the Slonczewski’s result[1] with spin polarization $P=1$ is also plotted in Fig. For CoCo/Al with $\theta > 60^\circ$ one can observe that our obtained $g(\theta)$ is barely affected by interfacial disorder and agrees well with the Slonczewski’s result. When $\theta$ is near $180^\circ$, our calculated $g(\theta)$ will divergence as the prediction of Slonczewski, except the value is smaller than Slonczewski’s result. Similarly, the $g(\theta)$ of MnSi/Al interface ($x \leq 0.2$) is also well consistent with Slonczewski’s result for $\theta > 60^\circ$. However, in contrast to the case of CoCo/Al, the $g(\theta)$ of MnSi/Al ($x \geq 0.3$) for $\theta > 60^\circ$ is significantly suppressed by interfacial disorder, especially for the case of $x = 0.5$. 

FIG. 4: (color online). The angular dependence of total in-plane STT on free CMS layer and total conductance of CMS/Al/CMS/Al SV system with different interfacial alloy concentration $x$. It is shown that for large interfacial alloy concentration x the torque (STT induced by unit bias) for MnSi/Al interface is approximately equal to that for CoCo/Al interface. The inset in figure (a) shows the concentration x dependence of the estimated asymmetry parameter $\Lambda$ of STT.
As is well known, the inverses of $g(0^\circ)$ and $g(180^\circ)$ are proportional to the critical current of switching out of the parallel and anti-parallel states for SV. From the inset of Fig. 3 one can see that the calculated $g(\theta)$ close to $\theta = 0^\circ$ are much larger than the prediction of Slonczewski for both CoCo/Al and MnSi/Al. Interestingly, in the case of MnSi/Al the $g(\theta)$ at small angle is even larger for disorder interface compared to the clean interface. In addition, one can also see that at $x = 0.5$ the $g(\theta)$ near $\theta = 0^\circ$ has still relatively large value for CoCo/Al ($g(10^\circ) \approx 0.47$) and for MnSi/Al ($g(10^\circ) \approx 0.55$). For the CMS/Al SV system, our calculations show that the maximum of $g(\theta)$ at small $\theta$ approaches to 0.7, which is about one order larger than the theoretical value of Co/Cu/Co SV [39]. Therefore, our calculated results suggest that the critical current of switching magnetization in SV can be significantly reduced using half-metal CMS as ferromagnetic layers.

Finally, to look the STT in CMS/Al SV a little further, we demonstrate the layer resolved STT with clean and disorder interface in Fig. 6. As expected, from Fig. 6 one can observe that the STT only exist around the interface region for both CoCo/Al and MnSi/Al. Moreover, it will decay very fast and almost disappear about 3-4 MLs away from the interface region, which indicates the spin angular momentum is totally absorbed by the interface in CMS/Al SV system. This behavior of layer resolved STT is very similar to the case of Fe/MgO/Fe tunnel junction [42], where the tunneling process is dominated by the half-metallic $\Delta_1$ state at $\Gamma$ point in Fe. Actually, in our CMS/Al/CMS SV system all the states which are responsible for transport have half-metallic nature, i.e. there is only propagating majority state in CMS while the minority state is evanescent. Therefore, as Heiliger and Stiles argued in Ref. 42, the rapid decay of STT away from CMS/Al interface can be attributed to the interference between the evanescent minority and propagating majority in half-metal CMS.
IV. SUMMARY

In summary, the STT of CMS/Al/CMS/Al(001) SV system with and without interfacial disorder have been studied by the noncollinear wave-function matching method based on TB-LMTO with ASA approximation. The obtained angular dependence of in-plane STT deviates from the symmetric sine function. For clean interface we estimate the asymmetry parameter $\Lambda \approx 4.5$ for CoCo/Al and $\Lambda \approx 2.9$ for MnSi/Al, which indicates that the CMS/Al-based high-frequency generators with clean CoCo/Al interface is much more efficient. Furthermore, the CMS/Al-based high-frequency generators with clean interface 62\[16\] J. Z. Sun, Phys. Rev. B \[11\] M. Oogane, T. Kubota, Y. Kota, S. Mizukami, H. Nakamura, M. Shirai, and T. Miyazaki, J. Magn. Magn. Mater. \[17\] M. Tsoi, A. G. M. Jansen, J. Bass, W.-C. Chiang, M. Seck, V. Tsoi and P. Wyder, Phy. Rev. Lett. \[12\] X. Q. Li, X. G. Xu, D. L. Zhang, X. G. Xu, J. Miao and Y. Jiang, Appl. Phys. Express \[10\] S. Mizukami, D. Watanabe, M. Oogane, Y. Ando, Y. Ito, H. Takahashi, H. Matsuoka and H. Ohno, IEEE Trans. Magn. \[13\] W. H. Wang, H. Sukegawa, H. Hasegawa, H. Matsuoka and H. Ohno, J. Solid-St. Circ. \[14\] N. Inami, H. Naganuma, M. Oogane, T. Nakanishi, Y. Ando, and K. Takanashi, Appl. Phys. Express \[15\] R. A. de Groot, F. M. Mueller, P. G. van Engen, and K. H. J. Buschow, Phys. Rev. Lett. \[16\] J. Z. Sun, Phys. Rev. B \[17\] M. Tsoi, A. G. M. Jansen, J. Bass, W.-C. Chiang, M. Seck, V. Tsoi and P. Wyder, Phys. Rev. Lett. \[18\] E. B. Myers, D. C. Ralph, J. A. Katine, R. N. Louie and R. A. Buhrman, Science 285, 867 (1999).

The efficiency parameter $g(\theta)$ at small $\theta$ are larger than the prediction of Slonczewski’s theory, where the maximum approaches to 0.7. It suggests that the half-metallic CMS is a very good candidate for STT-MRAM applications.

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