Effects of interfacial noncollinear magnetic structures on spin-dependent conductance in $Co_2MnSi/MgO/Co_2MnSi$ magnetic tunnel junctions: A first-principles study

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We investigate the effects of spin-flip scattering on tunneling magnetoresistance (TMR) in magnetic tunnel junctions (MTJs) with half-metallic Co_2MnSi (CMS) and MgO on the basis of the first-principles calculations. We found that noncollinear magnetic structures of interfacial Co spin moments resulting from the thermal fluctuations cause spin-flip scattering, leading to a significant reduction of the TMR. Interface states originating from a projection of the majority-spin Δ_1 states of CMS in the minority-spin half-metallic gap because of the interfacial noncollinear magnetic structures play an important role in the spin-flip process. From these results, together with an estimated interfacial exchange stiffness constant, we conclude that the TMR ratio at room temperature in MTJs with half-metallic Co-based full-Heusler alloys can be attributed to the spin-flip scattering by the interfacial noncollinear magnetic structures as a result of the thermal fluctuation.

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I. INTRODUCTION

The tunneling magnetoresistance (TMR) effect in magnetic tunnel junctions (MTJs) is essential for applications in spintronics, such as nonvolatile magnetic random access memories and the read-out head of hard-disk drives. One promising method of obtaining a huge TMR is the use of half-metallic ferromagnets (HMFs)[1] as ferromagnetic electrons in MTJs, in which the HMFs have a complete (100%) spin polarization at the Fermi level. In particular, Co-based full Heusler alloys (Co_2YZ)[2,3] are the most promising candidate for such applications because of their high Curie temperature (T_C) and robustness of high spin polarization against atomic disorder.[4–6] Many experiments on TMR have been performed for MTJs with Co_2YZ and an amorphous alumina barrier.[7–11] Furthermore, recent experiments on the TMR of MTJs with a Co_2YZ and MgO barrier have demonstrated large TMR ratios, the highest of which were over 700% at low temperatures, confirming the half-metallic character of Co_2YZ.[12–14] While large TMR ratios have been observed in MTJs with half-metallic Co_2YZ, these TMR ratios significantly decrease with increasing temperature.

To understand origin of the reduction of the TMR ratios at finite temperature, Lezaic *et al*. discussed the thermal collapse of spin polarization on the basis of a Monte Carlo method including results from the density functional theory (DFT).[15] They found that the spin polarization of bulk Co_2MnSi (CMS) decreased rapidly with increasing temperature for $T > 0.27T_C$ because of a change in hybridization due to spin fluctuation, where $T_C = 985$ K for CMS. Furthermore, Chioncel *et al*. investigated the effects of nonquasiparticle states appearing in the half-metallic gap of bulk CMS at finite temperatures using DFT calculations and the dynamical mean field theory.[16] They found that the total density of states (DOS) of CMS depends on temperature, leading to a significant reduction of the spin polarization at finite temperatures. To confirm the temperature dependence of the total DOS of bulk CMS, the valence-band electronic structures were investigated by photoelectron spectroscopy.[17] The experimental valence band photoemission spectra at 30 K were in good agreement with the DFT calculation results at zero temperature. Furthermore, no distinct temperature dependence was observed in the experimental valence band spectra. Therefore, the temperature dependence of the total DOS was rather weak compared to theoretical predictions.

Contrary to this, Mavropoulos *et al*. pointed out that interface states appearing in the half-metallic gap of HMFs contribute to spin-flip scattering through magnetic excitations at junctions with an insulating barrier, resulting in a reduction of the TMR at finite temperatures.[18] Furthermore, Sakuma *et al*. showed from the first-principles calculations that the exchange constant of interfacial Co spin moments at the CMS/MgO(001) interface is relatively small compared to that of bulk CMS, leading to instability of the interfacial Co spin moments at finite temperature.[19]

Therefore, to understand the origin of low TMR ratios at RT, it is essential to clarify the effects of spin-flip scattering at interfacial regions in MTJs. In this paper, we investigate the spin-dependent conductance of MTJs with CMS (or Fe) and MgO on the basis of the first-principles calculations in a noncollinear-spin system. Noncollinear magnetic structures are considered to be formed as a result of spin fluctuation at finite temperatures. We focus on the spin-flip scattering of conducting electrons caused by noncollinearity of the local spin moments in various interfacial layers and discuss the electronic states at the interfaces contributing to the spin-flip conductance. Our theoretical analysis confirmed the crucial contribution of spin-flip process at interfacial Co spin moments to the tunneling conductance of MTJs with antiparallel magnetization, which leads to a significant reduction of the TMR ratio at RT.

II. COMPUTATIONAL METHOD

We perform first-principles calculations for supercells consisting of CMS and MgO, using the DFT within the generalized-gradient approximation for the exchange-correlation energy.[20] In order to facilitate the optimization of atomic positions, which is important for determining the

interface structure, we adopt plane-wave basis sets along with the ultrasoft pseudopotential method by using the quantum code ESPRESSO.[21] The number of **k** points is taken to be $10 \times 10 \times 1$ for all cases, and Methfessel-Paxton smearing with a broadening parameter of 0.01 Ry is used. The cutoff energy for the wave function and charge density is set to 30 and 300 Ry, respectively. These values are large enough to deal with all the elements considered here within the ultrasoft pseudopotential method.

CMS/MgO/CMS(001) MTJs with Co (MnSi) termination were constructed in a multilayer containing 17 (15) atomic layers of CMS and 9 atomic layers of MgO (∼2 nm). The in-plane lattice parameter of the supercell is fixed at 3.99 Å. These values correspond to $a_0/\sqrt{2}$, where a_0 is the lattice constant of the bulk CMS (5.65 Å). Since the lattice constant of the rock salt MgO is 4.21 Å, the lattice mismatches between Co_2MnSi and MgO on the 45° in-plane rotation at the (001) face are 5.1%, which lead to 11.2% of tetragonal expansion in MgO.

Conductance calculations were implemented by the method of Choi and Ihm[22,23] that solves a scattering equation directly with a semi-infinite boundary condition to obtain the zero bias limit conductance at the Fermi level from the Landauer formula. The potential in the scattering equation can be obtained from the self-consistent electronic structure calculations in the collinear-spin system. The potential for a noncollinear-spin system was obtained by rotating the density matrix of a collinear-spin system with a spin-1/2 rotation matrix. According to Kübler's formulation,[24,25] off-diagonal elements of the effective potential that provides a spin mixing in the ballistic conductance are given by

$$\frac{1}{2}\left(\frac{\delta E_{\rm xc}}{\delta n_\uparrow} - \frac{\delta E_{\rm xc}}{\delta n_\downarrow}\right)(\sin\theta\cos\phi \pm i\sin\theta\sin\phi), \qquad (1)$$

where $\delta E_{\rm xc}/\delta n_{\rm s}$ (s $=\uparrow$, $\downarrow$) is the exchange and correlation potential in a collinear-spin system and θ and ϕ are polar and azimuthal angles of a local spin moment with respect to the global spin-quantum axis, respectively. Since our calculations neglected spin-orbit interaction, the azimuthal angle ϕ did not affect the calculation results and was set to zero. The off-diagonal part of the local potential expressed by Eq. (1) are given at real-space positions of the supercell within each atomic sphere of the interfacial atom having a noncollinear spin moment. Figure 1(a) shows the model system used for CMS/MgO/CMS MTJs with Co termination in the antiparallel magnetization, where the monolayer Co spin moments on both sides of the junction were canted by an angle θ in order to provide interfacial spin-flip scattering.

III. CALCULATION RESULT

Figure 1(b) shows the conductance of a CMS/MgO/CMS MTJ with Co termination in parallel or antiparallel magnetization as a function of the angle of the interfacial Co spin-moments. We obtained zero conductance at $\theta = 0°$ for antiparallel magnetization because of the half-metallic character of CMS. On the other hand, the antiparallel conductance increased with increasing θ, while the parallel conductance decreased. This behavior can be attributed to the spin-flip scattering because of the interfacial noncollinear magnetic

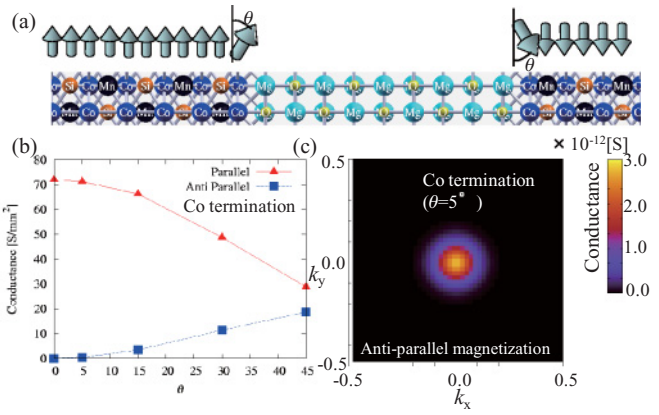

FIG. 1. (Color online) (a) Schematic figure of CMS/MgO/CMS MTJs with Co termination and local spin moments for each layer, with a noncollinear magnetic structure on both sides of the junction. (b) The parallel and antiparallel conductance of CMS/MgO/CMS MTJ as a function of the angle of interfacial local spin moments θ. (c) The in-plane wave-vector ($k_\parallel$) dependence of the antiparallel conductance of CMS/MgO(t)/CMS MTJ with $\theta = 5°$ for $t \sim 2.0$ nm (nine atomic layer of MgO).

structures. We show in Fig. 1(c) the in-plane wave-vector ($k_\parallel$) dependence of the tunneling conductance of the MTJ in the antiparallel magnetization with $\theta = 5°$. We have already shown in Refs. 26 and 27 that bulk CMS has a Δ_1 band at the Fermi level in the majority-spin states, and the $k_\parallel$-dependence of the conductance of CMS/MgO/CMS MTJs in the parallel magnetization has a broad peak at $k_\parallel = (0,0)$ because of the slow decay of Δ_1 states in the MgO barrier.[28] As can be seen in Fig. 1(c), the $k_\parallel$ dependence of the conductance in antiparallel magnetization also shows a broad peak at $k_\parallel = (0,0)$, indicating that the spin-flip conductance is dominated by the Δ_1 channel of the conducting electrons.

In Fig. 2, we show schematic images of the LDOS of interfacial Co atoms in collinear-spin ($\theta = 0$) and noncollinear-spin ($\theta \neq 0$) cases. In the case of collinear spin system, the CMS/MgO interface is not half metallic and has interface states in the half-metallic gap of minority-spin states originated from the nonbonding Co d orbital (see also Fig. 2 in Ref. 26). Then, the noncollinearity of interfacial Co spin-moments generates a spin-mixing in the LDOS of CMS/MgO/CMS(001). At the Fermi level, as is shown in Fig. 2(b), both bulk s states and interfacial Co d states are projected on the majority-spin and minority-spin states of the global spin-quantum axis, providing a spin-flip scattering of the ballistic conductance. The broad peak at $k_\parallel = (0,0)$ in Fig. 1(c) indicates that the projected minority-spin Δ_1 states mainly contribute to the conductance in antiparallel magnetization. This means that the contribution of the interfacial d states appearing at the Co termination of CMS/MgO junctions in the collinear-spin system [cross-hatched black areas in Fig. 2(a) and 2(b)] was rather small compared to that of the s states caused by the noncollinearity of interfacial Co spin moments [light-blue areas (light-gray areas in grayscale) in Fig. 2(b)]. Since the interface states were mainly composed of $d_{\rm xy}$ and $d_{\rm x^2-y^2}$ orbitals of interfacial Co atoms, they show the fast decay in the MgO barrier.

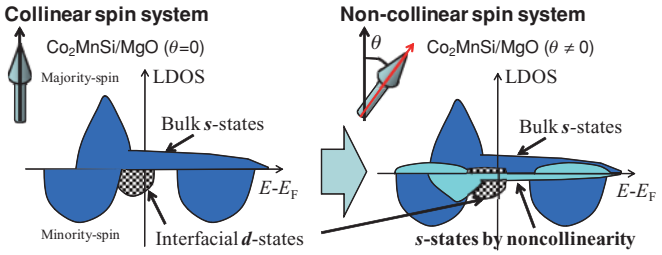

FIG. 2. (Color online) Schematic image of local density of states (LDOS) of interfacial Co atoms at Co_2MnSi (CMS)/MgO(001) junctions (a) for collinear spin ($\theta = 0$) and (b) for noncollinear spin ($\theta \neq 0$) cases. The blue areas (gray areas in grayscale), the cross-hatched black areas and the light-blue areas (light-gray areas in grayscale) indicate the LDOS for bulk CMS, for interfacial d-states, and for interfacial s-states by the noncollinear spin moments, respectively.

However, the contribution of interface states on the tunneling conductance depends on the barrier layer.[29] If the thickness of the MgO barrier is less than ≈1 nm, spin-flip conducting electrons through the interface states can contribute to the tunneling conductance. In Fig. 3, we show the $k_\parallel$ dependence of the tunneling conductance of the MTJ with five atomic layers of MgO ($t_{MgO} \approx 1$ nm) in the parallel and the antiparallel magnetization with $\theta = 5^\circ$. In the case of the parallel magnetization, the broad peak at $k_\parallel(0,0)$, which is a contribution from the Δ_1 states, surpasses the hot-spot peaks from the interfacial d states. Contrary to this, for the antiparallel conductance, we have obtained a hot-spot-like spiky structure because of the contribution of interface states. In this case, elimination of interface states at CMS/MgO junctions[27,30] in collinear-spin systems becomes important to reduce of the antiparallel conductance.

To examine the interfacial structure dependence of the spin-flip conductance, Fig. 4 shows logarithmic plots of TMR ratios as a function of the angle of local spin moment θ in various interfacial layers of CMS/MgO/CMS and Fe/MgO/Fe MTJs. First, we can confirm that the TMR ratios of the MTJs decreased with increasing θ because of spin-flip conductance at the interfacial region. In particular, the TMR ratios for CMS/MgO/CMS MTJs with the noncollinearity of interfacial and subinterfacial Co spin moments had similar values to that of Fe/MgO/Fe MTJs with $\theta > 5^\circ$. This indicates that the advantage of half-metallic electrodes is valid only for small θ if the noncollinearity arises at interfacial Co spin

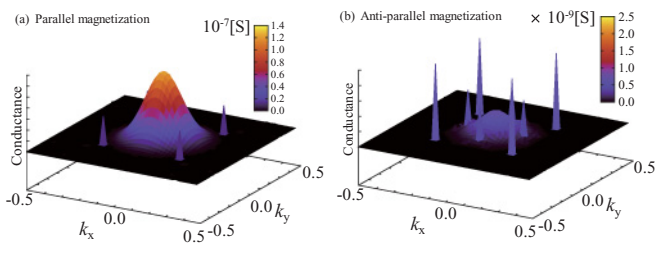

FIG. 3. (Color online) The in-plane wave-vector ($k_\parallel$) dependence of the (a) parallel and (b) antiparallel conductance of CMS/MgO(t)/CMS MTJ with $\theta = 5^\circ$ for $t \sim 1.0$ nm (five atomic layer of MgO).

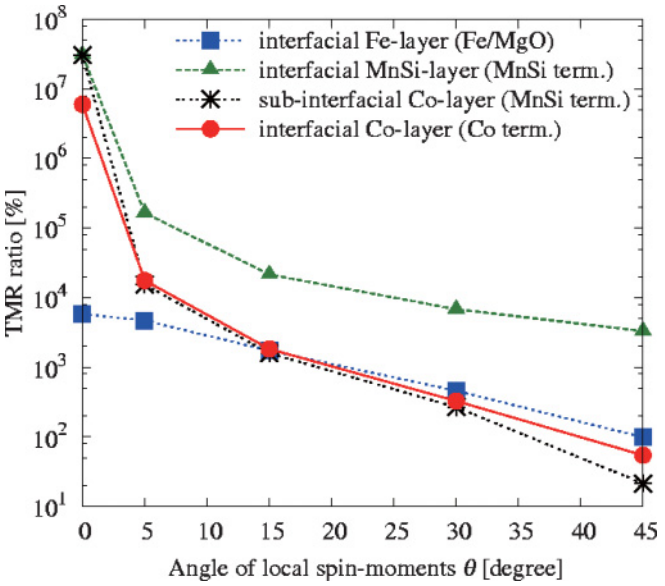

FIG. 4. (Color online) Logarithmic plots of TMR ratios as a function of the angle of local spin-moment θ for noncollinear magnetic structures of various interfacial layers in CMS/MgO/CMS MTJs and Fe/MgO/Fe MTJs.

moments. On the other hand, the decrease of the TMR ratio with increasing θ was rather gradual for MTJs with the noncollinearity of interfacial MnSi layers at MnSi termination compared to that of interfacial Co layers, indicating that the spin-flip conductance was suppressed at the interfacial MnSi layers. Since the Si atom is nonmagnetic, the off-diagonal part of the effective potential expressed by $(\delta E_{xc}/\delta n_\uparrow - \delta E_{xc}/\delta n_\downarrow)$ was rather small, which led to a suppression of the spin-flip probability at the MnSi layer. In our calculations, we neglect the angle dependence of the size of Co and Mn spin moments. This is reasonable approximation for Mn spin moments because of the localized character in bulk CMS[31,32] and MnSi-terminated interface.[33] For Co-terminated interface, the strong hybridization between Co and O atoms can cause the angle dependence of interfacial Co spin moments. As is discussed for Ni spin moments in NiMnSb,[34] the longitudinal fluctuation will increase the length of the local spin moments with increasing the angle. This will provide the enhancement of spin-flip scattering at interfacial regions, resulting in the further decrease of the TMR ratio.

To estimate the exchange stiffness of the interfacial spin moments, we calculated the increase of the one-electron band energy $E(\theta)$ relative to the collinear-spin system ($\theta = 0$). In Fig. 5, we have shown the $E(\theta)$ as a function of the angle of local moments θ for various interfacial layers in CMS/MgO(001) and Fe/MgO(001) junctions Then we fit these results using $E(\theta) = A(1-\cos\theta)$. Here A is the interatomic-layer exchange-stiffness constant, and we show the value in Table I for each layer in the interfacial and bulk regions. This estimation corresponds to the method of the magnetic force theorem.[35,36] We confirm that the increase of the band energy as a function of the canting angle shown in Fig. 5 can be fitted by $\sim\theta^2$ up to $\theta = 30^\circ$. This means that the error in the estimation of the exchange stiffness constant by the magnetic force theorem is very small in the present system.[37]

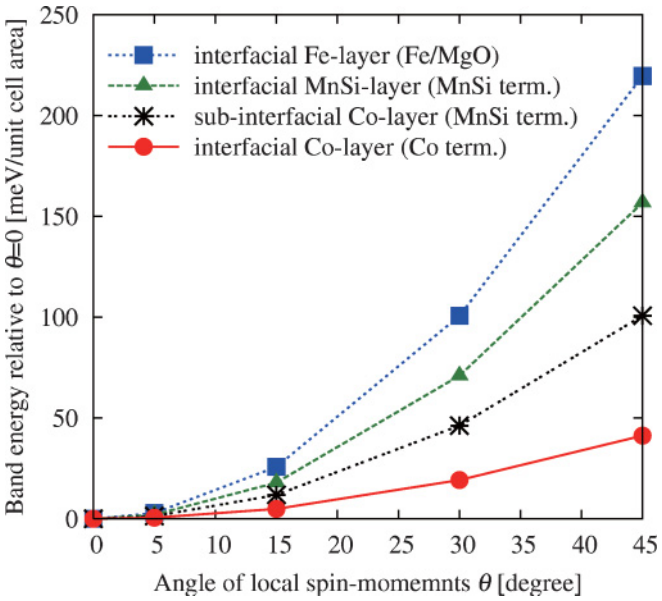

FIG. 5. (Color online) The increase of the band energy relative to that of the collinear-spin system $E(\theta)$ as a function of the angle of local spin moments θ for the various interfacial layers at CMS/MgO(001) and Fe/MgO(001) junctions.

First, we can find that the exchange stiffness of the interfacial Co layer at Co termination was much smaller than that of the interfacial MnSi layer at MnSi termination and that of bulk CMS. These results are consistent with the results of recent first-principles calculations of the exchange constant of CMS/MgO(001).[19] Furthermore, the exchange stiffness of the subinterfacial Co layer at MnSi termination was smaller than that of the interfacial MnSi layer. This means that at MnSi termination, the subinterfacial Co spin moments fluctuate more easily than interfacial Mn spin moments. On the other hand, we found a very high exchange stiffness of the interfacial Fe layer at Fe/MgO junctions compared to those of CMS/MgO junctions, indicating the robustness of interfacial Fe spin moments against thermal fluctuation. One possible reason for this behavior of the exchange stiffness at interfacial regions is related to a change in the interfacial spin moments compared to that of bulk CMS. As is discussed in Refs. 26 and 33, the majority-spin charge of interfacial Co atoms transfers to the MgO side because of the strong bonding between Co and O atoms. On the other hand, interfacial Mn spin moments of the CMS/MgO junction[27,33] and interfacial Fe spin moments of the Fe/MgO junction[38] increase in comparison with those of the bulk because of the localization effect (and band-narrowing effect) of the nonbonding d orbital in the interfacial regions. Since $E(\theta)$ can be characterized by the off-diagonal elements of the local potential expressed by Eq. (1), the decrease (increase) of local spin moments reduced (enhanced) the off-diagonal terms, leading to the low (high) exchange stiffness.

IV. DISCUSSION

Finally, we discuss the effect of interfacial spin-flip scattering on the TMR ratios of CMS/MgO/CMS and Fe/MgO/Fe MTJs at finite temperatures. To estimate the TMR ratio at a finite temperature, we calculated the Boltzmann average of the tunneling conductance using the following equation:

$$G_{\mathrm{P(AP)}}(T) = \int \frac{g_{\mathrm{P(AP)}}(\theta)\exp[-2E(\theta)/k_{\mathrm{B}}T]}{\exp[-2E(\theta)/k_{\mathrm{B}}T]}\sin\theta d\theta, \qquad (2)$$

where $g_{\mathrm{P(AP)}}(\theta)$ is the θ dependence of the tunneling conductance in parallel (P) and antiparallel (AP) magnetization, as shown in Fig. 1(b). $E(\theta)$ is the increase in the band energy caused by the noncollinearity of the local spin moments at each interfacial layer, as discussed in the previous paragraph. The factor of 2 for $E(\theta)$ indicates the contribution from both sides of the MTJs. By evaluating the tunneling conductance at finite temperature using Eq. (2), we obtained a TMR ratio of 700% at 300 K for CMS/MgO/CMS MTJs, including the thermal fluctuation of the interfacial Co spin moment at Co termination, and 1500% at 300 K for CMS/MgO/CMS MTJs, including the thermal fluctuation of the subinterfacial Co spin moment at MnSi termination. These TMR ratios were smaller than the TMR ratio of 2500% at 300 K for Fe/MgO/Fe MTJs, including the thermal fluctuation of the interfacial Fe spin moment, leading to the large temperature dependence of the TMR ratios for CMS/MgO/CMS MTJs compared to Fe/MgO/Fe MTJs. From these results, we can conclude that the experimentally observed low TMR ratio of the MTJs at RT can be attributed to the spin-flip conductance caused by thermal fluctuation of the interfacial spin moments. Therefore, to suppress the reduction of the TMR ratios at finite temperature in CMS/MgO/CMS MTJs, we must enhance the exchange stiffness of Co spin moments at the CMS/MgO(001) interface. In the estimation of the thermal average of the tunneling conductance, we treated $E(\theta)$ as the thermal excitation energy of the local spin moments, which corresponds to the replacement of various magnetic excitation modes at interfacial regions by a single excitation mode of interfacial spin moments given by $E(\theta)$. Furthermore, we fixed the angle of the local spin moments in neighboring layers in the evaluation of $E(\theta)$. Thus, there will be lower excitation mode of local spin moments at interfacial regions, and such a lower magnetic excitation will mainly contribute to the thermal average of the tunneling conductance at RT. However, the inclusion of the lower excitation energy in Eq. (2) leads to a further decrease in the TMR ratio at RT. Therefore, our conclusion that the significant reduction of the TMR ratio of CMS/MgO/CMS MTJs at RT can be attributed to the interfacial spin-flip conductance does not change with a more accurate estimation of the thermally averaged tunneling conductance.

TABLE I. Interlayer exchange stiffness constant A [meV/*uca*] fitted to the increase of the band energies $E(\theta) = A(1 - \cos\theta)$ by the noncollinearity of local spin moments for CMS/MgO(001) and Fe/MgO(001) junctions. (1st) and (2nd) indicate the first layer and the second layer at the interface with MgO, respectively. *uca* is the unit-cell area ~32 Å^2.

A (meV/*uca*)	Co (1st)	Co (2nd)	Mn (1st)	Fe (1st)
Bulk (CMS or Fe)	414	414	565	600
MgO interface	145	347	529	753

V. SUMMARY

In summary, we investigated the effects of spin-flip scattering by interfacial noncollinear magnetic structures on the TMR ratios of MTJs with CMS (or Fe) and MgO on the basis of the first-principles calculations. For Co-terminated CMS/MgO/CMS MTJs, the effects of the noncollinearity of interfacial Co spin moments on the TMR were significant, while the noncollinearity of interfacial Mn spin moments at the MnSi termination made a smaller contribution to the spin-flip conductance. The noncollinear magnetic structures at CMS/MgO junctions project the majority-spin Δ_1 states in the minority-spin states, producing the tunneling conductance through the MgO barrier in the antiparallel magnetization. Furthermore, the interatomic-layer exchange-stiffness constant of interfacial and subinterfacial Co spin moments at CMS/MgO junctions is much smaller than that of interfacial Mn spin-moments at CMS/MgO and Fe spin moments at Fe/MgO junctions. From these results, we conclude that the TMR ratio at room temperature in MTJs with half-metallic Co-based full-Heusler alloys can be attributed to the spin-flip scattering by the noncollinear magnetic structures of interfacial Co as a result of the thermal fluctuations. Our results demonstrate recent experimental results, that is, the significant reduction of the TMR ratios of CMS/MgO/CMS MTJs at room temperature compared to those of Fe/MgO/Fe MTJs. This means that the spin-flip scattering at the interface is at least as important as any other effect. Enhancement of the interfacial exchange stiffness by inserting an ultrathin Fe layer at CMS/MgO junctions will be effective to raise the TMR ratios at room temperature. The present findings suggest that TMR ratios of MTJs with half-metallic Co-based full-Heusler alloys at room temperature can be designed by controlling their junctions and that are worth further investigation.

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