Thermoelectricity and disorder of FeCo/MgO/FeCo magnetic tunnel junctions

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We compute the thermoelectric transport parameterized by the Seebeck coefficient and thermal/electric conductance of random-alloy FeCo/MgO/FeCo(001) magnetic tunnel junctions (MTJs) from first principles using a generalized Landauer-Büttiker formalism. The thermopower is found to be typically smaller than those of Fe/MgO/Fe(001) MTJs. The (magneto-)Seebeck effect is sensitive to the details of the FeCo/MgO interfaces. Interfacial can greatly enhance the thermoelectric effects in MTJs. We also compute angular-dependent Seebeck coefficients that provide additional information about the transport physics. We report large deviations from the Wiedemann-Franz law at room temperature.

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I. INTRODUCTION

Spin caloritronics is a research direction that provides alternative strategies for thermoelectric waste heat recovery and cooling by employing the spin degree of freedom [1,2]. Seebeck [3] and Peltier [4] effects in magnetic nanostructures become spin dependent, i.e., different spin channels contribute differently and can be modulated by the magnetization direction. Moreover, in magnetic heterostructures, a thermal spin transfer torque (TST) [5,6] can be induced by heat currents.

Magnetothermoelectric effects in magnetic tunnel junctions (MTJs) were measured recently [7–10], partly motivated by their potential applications in magnetic data storage technology since nanoscale heating has been realized for heat-assisted magnetic recording [11]. The reported Seebeck coefficients (*S*) in MgO-based MTJs vary from 22 μ V/K (Ref. [10]) to -770μ V/K (Ref. [8]) for similar barrier thicknesses, while for $\Delta S = S_p - S_{AP}$, the difference in Seebeck coefficients between magnetic parallel (P) and antiparallel (AP) configuration values between -8.7μ V/K (Ref. [7]) and -272μ V/K (Ref. [9]) were measured. Seebeck coefficients as high as mV/K have also been reported [12,13].

Due to the difficulty in determining the temperature difference across tunneling barriers, intrinsic Seebeck coefficients cannot be measured directly but have to be determined using thermal modeling, which introduces uncertainties. Calculations based on realistic electronic band structures yield Seebeck coefficients of less than $60 \,\mu V/K$ at room temperature (RT) [14,15].

The energy dependence of the MTJ conductance is sensitive to the band alignment between insulator and metal. The calculated thermoelectric coefficients depend quite sensitively on the chosen model, such as the absence or presence of defects in the barriers. In this paper, we address the complications introduced by disorder in the hope of approaching the experimental reality and find out how large the Seebeck coefficients might become by interface engineering.

Here we disregard any magnon contributions that govern, e.g., the spin Seebeck effect of magnetic insulators [16,17] to the thermoelectric properties, i.e., we assume that in metallic structures they are dominated by the mobile conduction electrons. We then may adopt the Landauer-Büttiker formalism as generalized to thermal transport and thermoelectric transport by Butcher [18], which treats electrical transport in terms of transmission through a scattering region between electron reservoirs. The Seebeck coefficient and thermal conductance by the mobile electrons can then be calculated from the energy-dependent conductance.

Here we combine the Landauer-Büttiker formalism for spin-polarized thermal and electrical transport with realistic electronic band structures to compute the Seebeck coefficient and thermal conductance in FeCo/MgO MTJs. In Sec. II, we present the details of the formalism. In Sec. III, the method is used to calculate the thermoelectric coefficients of FeCo/MgO/FeCo with perfect interfaces and in the presence of oxygen vacancies (OVs). In Sec. IV, we summarize our results.

II. THERMOELECTRIC COEFFICIENTS

We model a device sandwiched by left (L) and right (R) electron leads with chemical potential difference $\Delta \mu = \mu_{\rm L} - \mu_{\rm R}$ and temperature bias $\Delta T = T_{\rm L} - T_{\rm R}$. The heat flow \dot{Q} and electric current *I* then read [19]

$$\begin{pmatrix} \Delta \mu / (-e) \\ \dot{Q} \end{pmatrix} = \begin{pmatrix} R & S \\ \Pi & -\kappa \end{pmatrix} \begin{pmatrix} I \\ \Delta T \end{pmatrix},$$
 (1)

where *R* is the electrical resistance while Seebeck *S* and Peltier Π coefficients are related by the Onsager-Kelvin relation $\Pi = ST$.

The spin-dependent conductance

$$G_{\sigma} = \frac{e^2}{h} \int dE t_{\sigma}(E) [-\partial_E f(E)], \qquad (2)$$

where $\sigma = \uparrow (\downarrow)$ denotes the spin species, $t_{\sigma}(E)$ is the spin and energy (*E*)-dependent transmission probability, and the Fermi occupation $f(E) = f(E,\mu,T) = [e^{(E-\mu)/k_BT} + 1]^{-1}$, is a function of electrochemical potential $\mu = (\mu_{\rm L} + \mu_{\rm R})/2$ and temperature $T = (T_{\rm L} + T_{\rm R})/2$. In the linear response approximation, the total electric current reads

$$I(\Delta T, \Delta V)$$

$$= -\frac{e}{h} \sum_{\sigma} \int dE \left[f(E, \mu_{\rm L}, T_{\rm L}) - f(E, \mu_{\rm R}, T_{\rm R}) \right] t_{\sigma}(E)$$

$$\rightarrow \frac{e\Delta T}{hT} \sum_{\sigma} \int dE \left(E - \mu \right) \partial_E f(E) t_{\sigma}(E)$$

$$- \frac{e^2}{h} \Delta V \sum_{\sigma} \int dE \partial_E f(E) t_{\sigma}(E). \tag{3}$$

The Seebeck coefficient $S = -(\Delta V / \Delta T)_{I=0}$ is obtained by setting I = 0 in Eq. (3), leading to

$$S = -\frac{1}{eT} \frac{\sum_{\sigma} \int dE \left[(E - \mu)t(E)\partial_E f(E) \right]}{\sum_{\sigma} \int dEt(E)\partial_E f(E)}$$
$$= \frac{S_{\uparrow}G_{\uparrow} + S_{\downarrow}G_{\downarrow}}{G_{\uparrow} + G_{\downarrow}}, \tag{4}$$

where

$$S_{\sigma} = -\frac{1}{eT} \frac{\int dE \left[(E - \mu)t_{\sigma}(E)\partial_E f(E) \right]}{\int dE t_{\sigma}(E)\partial_E f(E)} , \qquad (5)$$

and $e = 1.602 \times 10^{-19}$ C. When the energy-dependent conductance varies slowly around the Fermi level, only the leading term in the Sommerfeld expansion contributes and Eq. (4) becomes

$$S \to -eL_0 T \partial_E \ln G(E)|_{E_f},\tag{6}$$

with Lorenz number $L_0 \equiv \pi^2 (k_B/e)^2/3 = 2.45 \times 10^{-8} \text{ V}^2 \text{ K}^{-2}.$

The electronic contribution κ to the thermal conductance is

$$\kappa \equiv -\left(\frac{Q}{\Delta T}\right)_{I=0} = -(K + S^2 G T), \tag{7}$$

where *K* in the Landauer-Büttiker formalism reads [18]

$$K = \frac{k_B^2 T}{e^2} \int dEG(E) \left(\frac{E-\mu}{k_B T}\right)^2 \partial_E f(E).$$

At low temperatures, the leading term in the Sommerfeld expansion K dominates and

$$K \to -L_0 T G(E_f). \tag{8}$$

We may disregard the term S^2GT when $S^2 \ll L_0$, which leads to the Wiedemann-Franz (WF) relation

$$\kappa \to -(L_0 + S^2)TG(E_f) \approx L_0TG(E_f).$$

The tunnel magnetoresistance (TMR) ratio is defined in terms of the conductances for P and AP configurations:

$$TMR = \frac{G_P - G_{AP}}{G_{AP}} \times 100\%, \tag{9}$$

where $G_{P/AP} = \frac{e^2}{h} \sum_{\sigma} t_{P/AP}^{\sigma}(E_f)$. Similarly, the tunnelmagneto-Seebeck (TMS) and tunnel magneto-heat-resistance (TMHR) ratios are defined as

TMS =
$$\frac{S_{\rm P} - S_{\rm AP}}{\min(|S_{\rm P}|, |S_{\rm AP}|)} \times 100\%$$
 (10)

and

$$\kappa_{\rm m} = \frac{\kappa_{\rm P} - \kappa_{\rm AP}}{\min\left(\kappa_{\rm P}, \kappa_{\rm AP}\right)} \times 100\%. \tag{11}$$

At sufficiently low temperature, the WF relation may be used in Eq. (11) and $\kappa_m \rightarrow TMR$.

III. THERMOELECTRICS OF FeCo/MgO/FeCo(001)

A. Model

We consider a two-terminal device consisting of a MgO barrier sandwiched by two semi-infinite ferromagnetic leads as shown in Fig. 1. Specifically, we address the $Fe_xCo_{1-x}/MgO/Fe_yCo_{1-y}$ random alloy system, where x, y are numbers between 0 and 1. The materials are in the bcc crystal structure and grown along the (001) direction. The atoms at the interfaces are not relaxed from their bulk crystal positions. OVs in MgO are energetically favorable because they relax the compressive strain at the interface during crystal growth [20]. We assume that OVs only exists in the first MgO atomic layers at the interfaces to FeCo.

The thermoelectric coefficients are governed by the energydependent conductance. While the lateral supercell method can be used to handle the impurity scattering in a metallic system [21], the required high accuracy of the energy-dependent conductance would be difficult to achieve, since the statistical error due to the disorder configurations is much larger for MTJs than metallic systems because of inefficient self-averaging in reciprocal space.

The coherent potential approximation (CPA) is more suitable for a quantitative analysis of transport through disordered tunnel junctions. We implemented the CPA into the Keldysh nonequilibrium Green-function formalism including nonequilibrium vertex corrections (NVC) [22]. The method has been generalized here to handle noncollinear magnetization textures. The details of the electronic structure and transport calculations can be found in Appendix A.

We use $4 \times 10^4 k$ points in the full two-dimensional (2D) Brillouin zone (BZ) to ensure numerical convergence. Our CPA method can only handle disorder in the scattering region; we use the virtual crystal approximation (VCA) to deal with the potential functions in the alloy leads. In order to prove that the VCA treats the FeCo electrodes with sufficient accuracy, we study the Fe/FeCo(6ML)/MgO(6ML)/FeCo(6ML)/Fe MTJs, including six monolayers (6ML) of the alloy FeCo into the



FIG. 1. (Color online) Schematic atomic structure of FeCo/ MgO/FeCo magnetic tunnel junctions. Disorder is modeled by randomly distributed oxygen vacancies in the MgO monolayer next to the FeCo/MgO interfaces. FeCo is a random alloy indicated by blue-magenta spheres; Mg: green spheres; O: red spheres. The O vacancies are indicated by yellow spheres.

TABLE I. TMR ratios of FeCo/MgO(nML)/FeCo with clean and dirty (5% OVs on both sides) interfaces for n = 3, 5, 7, and 9-ML-thick barriers, respectively.

n	Concentration	Disorder	TMR (%)
3	Fe _{0.25} Co _{0.75}	clean	577
	Fe _{0.50} Co _{0.50}	clean	934
	Fe _{0.75} Co _{0.25}	clean	1003
	Fe _{0.50} Co _{0.50}	5% OVs	209
5	Fe _{0.25} Co _{0.75}	clean	853
	Fe _{0.50} Co _{0.50}	clean	900
	Fe _{0.75} Co _{0.25}	clean	1017
	Fe _{0.50} Co _{0.50}	5% OVs	113
7	Fe _{0.25} Co _{0.75}	clean	902
	Fe _{0.50} Co _{0.50}	clean	957
	Fe _{0.75} Co _{0.25}	clean	1061
	Fe _{0.80} Co _{0.20}	clean	1178
	Fe _{0.50} Co _{0.50}	5%OVs	90
Expt. [9]	Co _{0.6} Fe _{0.2} B _{0.2}		\sim 70–140(RT)
Expt. [25]	Co _{0.2} Fe _{0.6} B _{0.2}		604(RT), 1144(5 K)
9	Fe _{0.25} Co _{0.75}	clean	947
	Fe _{0.50} Co _{0.50}	clean	1033
	Fe _{0.75} Co _{0.25}	clean	1101
	Fe _{0.50} Co _{0.50}	5% OVs	82
Expt. [7]	Fe _{0.50} Co _{0.50}		330(RT)

scattering region, thus treating them in the CPA. We compare the energy-dependent conductance with that computed for FeCo/MgO(6ML)/FeCo, in which the potential of the FeCo electrodes is treated by the VCA. Our calculations show that results are not sensitive to the approximate treatment of FeCo alloy electrodes and therefore we adopt this VCA in the following.

The TMR ratios calculated for barriers with different thicknesses are compared with experimental results in Table I. The thinnest MgO barrier that can currently be grown coherently comprises three ML [23,24]. In experiments [25], TMR ratios can be maximized through controlled annealing and other grow conditions, approaching our theoretical values for the clean interfaces. However, the samples used in the thermoelectric experiments [7,9] have lower TMR ratios and are most likely disordered in the form of \sim 3–5% OVs close to the interface.



FIG. 2. (Color online) Resistance-area (RA) dependence on the thickness of MgO barriers with clean (black squares) and disordered (with 5% OVs) (red circles) $Fe_{0.5}Co_{0.5}/MgO$ interfaces. The blue triangle and cyan star denote the experimental values.

In Fig. 2, we compare the computed resistance area (RA) with published experiments [9,26]. For 7-ML-thick MgO barriers (1.6 nm) in the parallel magnetic configuration, our calculation yields 23.8 $\Omega\mu m^2$ (clean) and 12 $\Omega\mu m^2$ (5% OVs), close to a measured 17 $\Omega\mu m^2$ for 1.5-nm-thick tunnel junctions [9].

B. Energy-dependent conductance $G_{\sigma}(E)$

Even though Fe/MgO/Fe and FeCo/MgO/FeCo MTJs appear very similar and have comparable large TMR ratios, their spectral conductance turns out to be quite different. In Fe-based MgO MTJs, resonant transmission channels exist just below the Fermi level [6], which are not found for FeCo contacts. Figure 3 shows the spectral conductance of Fe_{0.5}Co_{0.5}/MgO(5ML)/Fe_{0.5}Co_{0.5} (001) MTJs with a given concentration of OVs at both interfaces for P and AP magnetic configurations. The energy window in the plots corresponds to 11 k_BT at room temperature (300 K), where k_B is the Boltzmann constant. The slope of the energy-dependent



FIG. 3. (Color online) Energy-dependent conductance of $Fe_{0.5}Co_{0.5}/MgO(5ML)/Fe_{0.5}Co_{0.5}$ with clean (green hollow squares), 5% OVs (yellow squares), 7.5% OVs (red circles), 10% OVs (blue triangles) at both interfaces for P and AP configurations.



FIG. 4. (Color online) Energy-dependent conductance for minority-spin channel in Fe_{0.5}Co_{0.5}/MgO(5ML)/Fe_{0.5}Co_{0.5} MTJs with interfaces that are clean (black squares) or contain 5% OVs (red circles) or 10% OVs (blue up-triangles), respectively, for the P configurations. Inset: Energy-dependent conductance for the minority-spin channel in Fe_xCo_{1-x}/MgO(5ML)/Fe_xCo_{1-x} MTJs with different alloy concentrations x = 1 (black squares), 0.9 (red circles), 0.7 (blue up-triangles), and 0.5 (green down-triangles), respectively, but without OVs.

transmission around the Fermi energy dramatically changes by only small amounts of OVs for P and AP.

Results for a wider energy window of $E = E_f \pm 1.2 \text{ eV}$ are given in Fig. 4. Two peaks are observed above the Fermi level for the minority spins. The OVs broaden these peaks and shift them towards the Fermi level, where they increase the conductance.

Thermoelectric effects are closely related to the slope of the energy-dependent conductance near the Fermi level. Clearly a certain amount of OVs at FeCo/MgO interfaces can enhance the Seebeck and Peltier coefficients.

The origin of these two peaks is not easy to identify for MTJs with random alloys. Fortunately, similar conductance peaks also exist in epitaxial Fe/MgO/Fe. The energydependent conductance for epitaxial Fe/MgO(5ML)/Fe (inset of Fig. 4, x = 1, black squares) displays a peak at 1.15 eV above the Fermi energy and a shoulder around 0.9 eV. The shoulder then develops into a plateau with 10% Co atoms added (red circles). At higher Co concentrations (x = 0.7, 0.5), the plateau develops into a second peak that shifts downwards to the Fermi level, where it affects the thermoelectric properties.

We can identify the origin of these features in epitaxial Fe/MgO/Fe by plotting the k_{\parallel} -resolved transmission for the minority spin in Fe/MgO(5ML)/Fe at different energies (see Fig. 5). We observe "hot" single or double rings with energy-dependent diameters. The maximum transmission approaches unity, indicating resonant tunneling through the barrier. A detailed study (see Appendix B) reveals that the single rings at lower energy ($E_f + 0.7 \text{ eV}$) can be identified to be bonding orbitals of low-energy interface states on both sides of the barrier. The corresponding antibonding states show up as the inner



FIG. 5. (Color online) k_{\parallel} -resolved transmission of minority spins through Fe/MgO(5ML)/Fe(001) MTJs in the P configurations with clean interfaces for different energies above the Fermi level.

rings at higher energy, which coexist with the bonding orbital of two higher-energy interface states that form the outer rings.

C. Seebeck coefficient

We limit the integration in Eq. (4) that defines the Seebeck coefficient to the interval $E - E_f \in (-0.3, 0.3)$ eV, introducing errors of less than 0.5% at T = 300 K (RT). Figure 6 shows our results for the Seebeck coefficient at RT of Fe_{0.5}Co_{0.5}/MgO(5ML)/Fe_{0.5}Co_{0.5} MTJs with various (but equal) concentrations of OVs at both FeCo/MgO interfaces. The clean interface (black squares) gives the smallest Seebeck coefficient, while an increasing OV concentration (up to 10%, blue down-triangles) enhances it by an order of magnitude for the P configuration. We can understand the enhanced thermoelectricity by the spectral conductance in the vicinity of the Fermi level that reflects the downward energy shift of the resonant tunneling states by the interface disorder. We eventually may take advantage of this insight to engineer thermoelectric effects. The magneto-Seebeck ratio $S_{\rm m}$, on the other hand, is larger for the ordered system, viz., 369.3% and -3.6% for clean and 10% OVs, respectively.

We list Seebeck coefficients and the corresponding magneto-Seebeck ratios for different MgO barrier thicknesses



FIG. 6. (Color online) Seebeck coefficients of $Fe_{0.5}Co_{0.5}/MgO(5ML)/Fe_{0.5}Co_{0.5}$ MTJs with clean interfaces (black squares), 5% (red circles), 7.5 % (green up-triangles), 10% OVs (blue down-triangles) at both interfaces.

TABLE II. Seebeck coefficients (in unit of $\mu V/K$) and magneto-Seebeck ratios TMS (in %) of Fe_{0.5}Co_{0.5}/MgO(*n*ML)/Fe_{0.5}Co_{0.5} MTJs at T = 300 K for P and AP, compared with experimental results from Ref. [7].

n	Disorder	Р	AP	<i>S</i> _m (%)
3	clean	-2.09	-23.82	1039.7
	5% OVs	-6.93	-19.41	180.1
	7.5% OVs	-12.87	-16.65	29.4
	10% OVs	-14.78	-25.77	74.4
5	clean	-8.08	-37.92	369.3
	5% OVs	-22.48	-52.79	134.8
	7.5% OVs	-55.80	-69.23	24.1
	10% OVs	-77.36	-74.70	-3.6
7	clean	-15.13	-50.26	267.6
	5% OVs	-40.46	-76.44	88.9
	7.5% OVs	-101.33	-99.20	-2.2
	10% OVs	-124.93	-98.93	-26.3
9	clean	-23.12	-61.50	166.0
	5% OVs	-62.79	-99.80	58.9
	6.5% OVs	-112.86	-119.05	8.4
	7% OVs	-132.10	-124.15	-6.4
	7.5% OVs	-149.17	-127.99	-16.5
	10% OVs	-155.79	-121.74	-30.0
Expt. [7]		-107.9	-99.2	-8.8

in Table II. First, the Seebeck coefficient increases with thicker MgO barriers with identical interface disorder for both the P and AP. For example, the Seebeck coefficient of MTJs with MgO(9ML) is \sim 2–10 times larger than that of MgO(3ML) for different interfacial quality and configurations, while the conductance changes by five orders of magnitude. The Seebeck coefficient is therefore much less sensitive to the MgO barrier thickness than the conductance. Second, at RT, the sign of the Seebeck coefficient does not change with thickness and its value is enhanced by OVs at the interface. In our study, the thermopower is maximized for 10% OVs for 5ML MgO, which can be understood from the spectral conductance in Fig. 4. Third, the order and sign of the magneto-Seebeck ratio TMS is sensitive to the details of the interfacial roughness. In Table II and Fig. 3, we see that when the interface is clean, $|S_{AP}| > |S_P|$, so the TMS is large and positive. Both $S_{\rm P}$ and $S_{\rm AP}$ increase when the interfaces are disordered by OVs, but S_P always grows faster than S_{AP} , which can be seen by inspecting the slopes around the Fermi level in Fig. 3. So the TMS decreases and even may change sign at low temperatures, especially when the TMS at RT is small.

Our calculation of Seebeck coefficients and the TMS of 9ML MgO barriers with 7% OVs at the interfaces are consistent with the experiment results [7] in Table II for P and AP, respectively.

In Table II, we show that MTJs with nine monolayers MgO have the largest Seebeck coefficient. However, its conductance and therefore thermoelectric current $GS\Delta T$ is small. The thinnest MgO junctions therefore still generate the largest thermoelectric power for a given temperature difference.

 S_P in Fe/MgO(5ML)/Fe with clean interfaces is 17.8 μ V/K at RT; the value is large than that of FeCo/MgO(5ML)/FeCo as -8.08μ V/K.



FIG. 7. (Color online) Angle-dependent Seebeck coefficient of $Fe_{0.5}Co_{0.5}/MgO/Fe_{0.5}Co_{0.5}$ without OVs at 300 K (black squares), 150 K (red circles), and 80 K (blue up-triangle).

The angular-dependent Seebeck coefficient (ADS) and conductance can provide additional information about the transport process. We plot the computed ADS at 300 K (black squares), 150 K (red circles), and 80 K (blue triangles) for Fe_{0.5}Co_{0.5}/MgO(5ML)/Fe_{0.5}Co_{0.5} in Fig. 7. The horizontal axis denotes the relative angle between magnetizations. The Seebeck coefficient varies slowly from P (0°) to 90° and drastically from 90° to the AP (180°), consistent with a previous report [27]. Deviations from the simple $\cos \theta$ dependence [28] illustrate the importance of multiple scattering in the barrier consistent with the existence of resonant states.

D. Thermal conductance κ

The electronic heat conductance is governed by the symmetric component of the spectral conductance around the Fermi level. Figure 8 shows the thermal conductance of $Fe_{0.5}Co_{0.5}/MgO(5ML)/Fe_{0.5}Co_{0.5}(001)$ with 0%, 5%, 7.5%, and 10% OVs at both interfaces, respectively. The thermal conductance is enhanced by the OVs for the same reasons as the charge conductance and Seebeck coefficient are. 10% OVs enlarge the thermal conductance by 5 and 33 times for the P and AP compared to clean interfaces at RT, respectively. The tunnel magneto-heat-resistance (TMHR) ratio is strongly modified by the OVs at the interface: we find 744.4% and 23.3% for clean and 10% OVs at both interfaces, respectively.

At sufficiently low temperatures, the Wiedemann-Franz (WF) law always holds. When S^2 becomes large, we have to consider the Seebeck-Peltier effect on the heat conductance (for constant ΔT). When the thermal conductance varies significantly in the thermal window k_BT , the Sommerfeld approximation breaks down and the WF relation is no longer valid. The calculated deviations from the WF law are plotted in Fig. 8. We define an effective Lorenz number $L_{\rm eff}$ by

$$\kappa = L_{\rm eff} T G \left(E_f \right), \tag{12}$$



FIG. 8. (Color online) Temperature-dependent thermal conductances for $Fe_{0.5}Co_{0.5}/MgO(5ML)/Fe_{0.5}Co_{0.5}$ with clean interfaces as well as 5%, 7.5%, and 10% OVs at both interfaces. The open symbols denote the heat conductances expected from the Wiedemann-Franz (WF) Law.

to emphasize the breakdown of the WF law by comparing L_{eff} with the Lorenz constant $L_0 = 2.45 \times 10^{-8} \text{ V}^2 \text{ K}^{-2}$. The temperature-dependent effective Lorenz number for different OV concentrations is shown in Fig. 9. For elevated temperatures, L_{eff} is found to be significantly enhanced compared to L_0 . The thermal conductance and corresponding TMHR ratios for different MgO barriers are listed in Table III. First, the thermal conductance decreases sharply with thicker MgO for both P and AP. Second, the thermal conductance is enhanced by interfacial OVs, whereas the TMHR ratios decrease. Third, the TMHR ratio is less sensitive to interfacial disorder for thicker MgO barriers. Large deviations from the WF law at RT are induced by OVs and calculated thermal conductance



FIG. 9. (Color online) Effective Lorenz number $L_{\rm eff}$ of Fe_{0.5}Co_{0.5}/MgO(5ML)/Fe_{0.5}Co_{0.5}(001) with clean interfaces and 5%, 7.5%, and 10% OVs at both interfaces.

TABLE III. Thermal conductance (in units of $10^6 \text{ Wm}^{-2} \text{ K}^{-1}$) and κ_m (%) of Fe_{0.5}Co_{0.5}/MgO(*n*ML)/Fe_{0.5}Co_{0.5} MTJs at T = 300 K for P and AP configurations with different interfacial roughness. The corresponding WF law values are shown in parentheses.

n	Disorder	Р	AP	κ _m
3	clean	128.67 (135.4)	16.44 (15.0)	682.7
	5% OVs	147.26 (145.7)	55.28 (46.6)	166.4
	7.5% OVs	169.9 (163.5)	84.1 (70.5)	102.1
	10% OVs	198.13 (197.6)	122.99 (102.5)	61.1
5	clean	4.56 (4.58)	0.54 (0.46)	744.4
	5% OVs	7.35 (6.20)	4.15 (2.89)	77.1
	7.5% OVs	12.77 (8.41)	9.17 (6.09)	39.3
	10% OVs	22.03 (16.25)	17.86 (13.36)	23.3
7	clean	0.313 (0.307)	0.037 (0.030)	737.8
	5% OVs	0.84 (0.61)	0.53 (0.32)	58.5
	7.5% OVs	2.27 (1.08)	1.59 (0.91)	42.8
	10% OVs	5.73 (3.35)	4.15 (2.97)	38.1
9	clean	0.027 (0.026)	0.003 (0.002)	800.0
	5% OVs	0.137 (0.083)	0.087 (0.045)	57.5
	7.5% OVs	0.581 (0.208)	0.383 (0.187)	51.7
	10% OVs	2.364 (1.127)	1.552 (1.016)	52.3

is larger than expected from the WF law. The numbers in parentheses in Table III are the WF values for *n*ML MgO with OVs. The calculated heat conductance deviates $\sim 18\%-51\%$ from the WF law at RT.

IV. SUMMARY

In conclusion, we computed the thermoelectric coefficients of FeCo/MgO/FeCo MTJs from first principles. Controlled oxygen vacancies in MgO close to the interface to FeCo can be used to engineer thermoelectric effects. While interface disorder can greatly increase the Seebeck coefficient, it suppresses the magneto-Seebeck ratio. The vacancy concentration is therefore an important design parameter in switchable thermoelectric devices based on magnetic tunnel junctions.

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APPENDIX A: COHERENT POTENTIAL APPROXIMATION (CPA) FOR TRANSPORT IN NONCOLLINEAR MAGNETIC SYSTEMS

In Ref. [22], Ke *et al.* formulated the nonequilibrium vertex correction (NVC) in the CPA in order to calculate disorder averaging at finite voltage bias in two-probe devices. When the direction of the magnetization changes slowly in space, the local electronic potentials should not be modified significantly

from a collinear magnetic system. We may then employ the frozen potential approximation to generalize the NVC theory to noncollinear magnetization textures.

Let us start with the "tail-cancellation" equation in the tightbinding linear muffin-tin orbital, atomic sphere approximation (TB-LMTO-ASA) framework:

$$\det\left[\mathcal{P}_{\mathcal{RL}}^{\alpha} - U_{\mathcal{R}}^{\dagger} S_{\mathcal{RL},\mathcal{R}'\mathcal{L}'}^{\alpha} U_{\mathcal{R}'}\right] = 0, \qquad (A1)$$

in which the coherent potential functions \mathcal{P}^{α} contain all information about the disorder and S^{α} is the structure constant, while the superscript α indicates screening. The subscript \mathcal{R} denotes the atom site and $\mathcal{L} \equiv (l,m)$ is the orbital index. The unitary rotation matrix $U_{\mathcal{R}}$ is

$$U_{\mathcal{R}}(\theta_{\mathcal{R}},\varphi_{\mathcal{R}}) = \begin{bmatrix} \cos\frac{\theta_{\mathcal{R}}}{2}e^{-i\frac{\varphi_{\mathcal{R}}}{2}} & -\sin\frac{\theta_{\mathcal{R}}}{2}e^{-i\frac{\varphi_{\mathcal{R}}}{2}}\\ \sin\frac{\theta_{\mathcal{R}}}{2}e^{i\frac{\varphi_{\mathcal{R}}}{2}} & \cos\frac{\theta_{\mathcal{R}}}{2}e^{i\frac{\varphi_{\mathcal{R}}}{2}} \end{bmatrix}, \quad (A2)$$

where $\theta_{\mathcal{R}}, \varphi_{\mathcal{R}}$ are the polar angles of the local magnetization direction. The screened structure constants $S^{\alpha}_{\mathcal{RL},\mathcal{R}'\mathcal{L}'}$ in Eq. (A1) are block diagonal matrices in spin space and depend only on the crystal structure,

$$S^{\alpha}_{\mathcal{RL},\mathcal{R}'\mathcal{L}'} \equiv \begin{bmatrix} s^{\alpha}_{\mathcal{RL},\mathcal{R}'\mathcal{L}'} & 0\\ 0 & s^{\alpha}_{\mathcal{RL},\mathcal{R}'\mathcal{L}'} \end{bmatrix}, \quad (A3)$$

and we define

$$\tilde{S}^{\alpha}_{\mathcal{RL},\mathcal{R}'\mathcal{L}'} = U^{\dagger}_{\mathcal{R}} S^{\alpha}_{\mathcal{RL},\mathcal{R}'\mathcal{L}'} U_{\mathcal{R}'}.$$
(A4)

Only the scattering region contains disorder. Each atomic position in the alloy as well as barrier can be occupied by two atomic species, Q = A, B, with concentration $C_{\mathcal{R}}^A$ and $C_{\mathcal{R}}^B$ ($C_{\mathcal{R}}^A + C_{\mathcal{R}}^B = 1$). The conditionally averaged auxiliary Green's function is introduce as [30]

$$\overline{g}^{\alpha} = \overline{[P^{\alpha} - \tilde{S}^{\alpha}]^{-1}} = [\mathcal{P}^{\alpha} - \tilde{S}^{\alpha}]^{-1}, \qquad (A5)$$

where $\overline{[\cdot]}$ is an average over random disorder configurations. The coherent potential function $\mathcal{P}_{\mathcal{R}}^{\alpha}$ satisfies the self-consistent relation [22]

$$\mathcal{P}_{\mathcal{R}}^{\alpha} = \overline{P}_{\mathcal{R}}^{\alpha} + \left(\mathcal{P}_{\mathcal{R}}^{\alpha} - P_{\mathcal{R}}^{\alpha,A}\right)\overline{g}_{\mathcal{R}\mathcal{R}}^{\alpha}\left(\mathcal{P}_{\mathcal{R}}^{\alpha} - P_{\mathcal{R}}^{\alpha,B}\right), \quad (A6)$$

where $\overline{P}_{\mathcal{R}}^{\alpha} = (C_{\mathcal{R}}^{A} P_{\mathcal{R}}^{\alpha,A} + C_{\mathcal{R}}^{B} P_{\mathcal{R}}^{\alpha,B})$ and $P_{\mathcal{R}}^{\alpha,Q}$ is the screened potential function of atomic species Q at \mathcal{R} .

The transmission probability through the system is [22]

$$\mathbf{T} = \operatorname{tr} \left[\Gamma_L \overline{g_{cc,1N}^{\alpha,r}} \Gamma_R g_{cc,N1}^{\alpha,a} \right], \tag{A7}$$

where $\overline{g}_{cc,N1}^{\alpha,a} = (\overline{g}_{cc,1N}^{\alpha,r})^{\dagger}$ and subscript *cc* denotes the central region. The transport system is always partitioned into principle layers (PL) indexed by $p = \ldots, -1, 0, 1, \ldots, N - 1, N, N + 1, \ldots$ The central region contains *N* layers where $p = 1, \ldots, N$. $\Gamma_{L/R}$ is the spectral function matrix of the ordered left/right leads. The trace runs over atom sites and orbitals.

The configurational average in Eq. (A7) can be expressed as

$$\overline{[g^{\alpha,r}\Gamma_{R}g^{\alpha,a}]} = \overline{g}^{\alpha,r}\Gamma_{R}\overline{g}^{\alpha,a} + \overline{g}^{\alpha,r}\Omega^{\alpha}_{NVC}\overline{g}^{\alpha,a}, \quad (A8)$$

where

$$\Omega_{\rm NVC}^{\alpha} = \sum_{\mathcal{R}} \Omega_{\rm NVC,\mathcal{R}},\tag{A9}$$

and

$$\Omega_{\text{NVC},\mathcal{R}} = \sum_{Q=A,B} C_{\mathcal{R}}^{Q} t_{\mathcal{R}}^{Q,r} [\overline{g}^{\alpha,r} \Gamma_{R} \overline{g}^{\alpha,a}]_{\mathcal{R}\mathcal{R}} t_{\mathcal{R}}^{Q,a} + \sum_{Q=A,B} C_{\mathcal{R}}^{Q} t_{\mathcal{R}}^{Q,r} \left[\overline{g}^{\alpha,r} \sum_{\mathcal{R}' \neq \mathcal{R}} \Omega_{\text{NVC},\mathcal{R}'} \overline{g}^{\alpha,a} \right]_{\mathcal{R}\mathcal{R}} t_{\mathcal{R}}^{Q,a},$$
(A10)

where

$$t_{\mathcal{R}}^{\mathcal{Q},r} = \left(\mathcal{P}_{\mathcal{R}}^{\alpha} - P_{\mathcal{R}}^{\alpha,\mathcal{Q}}\right) \left[1 - \overline{g}_{\mathcal{R}\mathcal{R}}^{\alpha,r} \left(\mathcal{P}_{\mathcal{R}}^{\alpha} - P_{\mathcal{R}}^{\alpha,\mathcal{Q}}\right)\right]^{-1}, \quad (A11)$$

with $t_{\mathcal{R}}^{Q,r} = (t_{\mathcal{R}}^{Q,a})^{\dagger}$. Finally, the transmission probability can be written

$$\mathbf{T} = \operatorname{tr}\left[\Gamma_{L}\overline{g}_{cc,1N}^{\alpha,r}\Gamma_{R}\overline{g}_{cc,N1}^{\alpha,a}\right] + \operatorname{tr}\left[\Gamma_{L}\overline{g}_{cc,1N}^{\alpha,r}\Omega_{NVC}\overline{g}_{cc,N1}^{\alpha,a}\right],$$
(A12)

where Ω_{NVC} is the noncollinear vertex correction. The first term on the right-hand side of Eq. (A12) corresponds to specular and the second to diffusive scattering, respectively.

APPENDIX B: ANALYSIS OF THE RESONANT "HOT" RINGS

The bonding and antibonding states originate from two localized interface states that couple to each other through the thin tunnel barrier [29]. The antibonding state with a node in the center of the barrier is shifted to higher energy, while the bonding state at lower energy should have a finite electron density in the barrier. Bonding and antibonding states can therefore be identified by the layer-resolved density of states (DOS).

Grouping atoms into layers, the equation of motion (EOM) for the *I*th layer can be written as [21]

$$-\mathcal{S}_{I,I-1}\mathbf{C}_{I-1} + [\mathcal{P}(E) - \mathcal{S}]_{II}\mathbf{C}_{I} - \mathcal{S}_{I,I+1}\mathbf{C}_{I+1} = 0, \quad (B1)$$

where *E* is the energy and \mathbb{C}_I is the wave-function amplitude in the localized orbital basis $|\mathcal{RL}\rangle$. The EOM with open boundary conditions for a device usually contains an infinite number of equations. By incorporating the boundary conditions in the leads, the scattering problem can be reduced to a set of coupled linear equations with finite number of equations and the scattering wave function can be found as

$$\begin{pmatrix} \mathbf{C}_{0} \\ \mathbf{C}_{1} \\ \mathbf{C}_{2} \\ \vdots \\ \mathbf{C}_{I} \\ \mathbf{C}_{I+1} \end{pmatrix} = (\mathcal{P} - \tilde{\mathcal{S}})^{-1} \\ \times \begin{pmatrix} S_{1,-1} \left[F_{L}^{-1} \left(+ \right) - F_{L}^{-1} \left(- \right) \right] \mathbf{C}_{0} \left(+ \right) \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \quad (B2)$$

where \tilde{S} is a block tridiagonal matrix with $\tilde{S}_{0,0}$ and $\tilde{S}_{I+1,I+1}$ renormalized by the boundary condition to the leads.

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FIG. 10. (Color online) Schematic atomic structure of Fe/MgO(5ML)/Fe magnetic tunnel junctions; the numbers are the numbers I of the atom layers used below.

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TABLE IV. Energies (in units of eV) of bonding and antibonding states in Fe/MgO(5ML)/Fe(001) MTJs. The energy splitting $\Delta E = E_{\text{antibonding}} - E_{\text{bonding}}$ reflects their overlap and is a function of energy.

$E_{\text{bonding}} - E_f$	0.5	0.6	0.7	0.8	0.9	1.0
$E_{\text{anti-bonding}} - E_f$	0.916	0.972	1.012	1.067	1.104	1.148
$\Delta E (\text{eV})$	0.416	0.372	0.312	0.267	0.204	0.148





FIG. 11. (Color online) (a1), (b1) Transmission spectrum in 2D BZ $[k_{\parallel} = (k_x, k_y) \in (\pm \frac{\pi}{a}, \pm \frac{\pi}{a})$, and *a* is the lattice constant] at energy $E_1 = E_f \pm 0.7$ eV and $E_2 = E_f \pm 1.012$ eV, respectively. (a2), (b2) Three-dimensional (3D) plots of $\rho = \rho_I(k_{\parallel})$ (arb. units) for Fe/MgO(5ML)/Fe MTJs, where $k_{\parallel} = (k_x, k_y)$ corresponds to the white square in (a1): $k_{\parallel} \in (\pm 0.24, \pm 0.24)\frac{\pi}{a}$; (b1): $k_{\parallel} \in (\pm 0.32, \pm 0.32)\frac{\pi}{a}$. (a3) DOS of typical k_{\parallel} points on the single "hot" ring. (b3), (b4): DOS of typical k_{\parallel} points on the inner and outer hot rings in (b1).



FIG. 12. (Color online) k_{\parallel} -resolved transmission probabilities of minority spins through Fe/MgO(5ML)/Fe(001) MTJs in the P configurations with clean interfaces and for various energies. The white arrows map the inner ring (antibonding state) at high energy on the single ring (bonding state) at low energy with the same radius.

Let us consider an electronic Bloch wave with amplitude $C_0(+)$, where +/- in the bracket denotes right/left-going components. Equation (B2) gives us the wave-function amplitudes of layers from 0 to I + 1 as well as the wave functions $\mathbf{a}_I = \Delta_I^{-\frac{1}{2}} \mathbf{C}_I$, where Δ is a potential parameter called the width of the \mathcal{RL} th "band" [30,31]. All of the physical quantities in Eq. (B2) are $k_{||}$ resolved in our calculations, and $\rho_I(k_{||}) = \mathbf{a}_I^{\dagger}(+,k_{||})\mathbf{a}_I(+,k_{||})$, where $\mathbf{a}_I(+,k_{||})$ is the right-going components of scattering wave function. We label the monolayers of the MTJ as shown in Fig. 10.

We first focus on the resonant tunneling "hot" ring at $E_1 = E_f + 0.7$ eV shown in Fig. 11(a1). The transmission probability on the ring approaches unity. By scanning the energy-dependent transmission probability for the $k_{||}$ on this ring, we find a ring with the same radius at $E_2 = E_f + 1.012$ eV, i.e., the inner ring in Fig. 11(b1). This ring is now accompanied by a second one with larger radius.

To identify the origin of these rings, we plot $\rho_I(k_{||})$ for the two energies in Figs. 11(a2) and 11(b2), where $k_{||} = (k_x, k_y)$ corresponds to the white squares in Figs. 11(a1) and 11(b1), respectively. The DOS is concentrated on the rings, where it is enhanced on the Fe atoms next to the interfaces.

Figures 11(a3), 11(b3), and 11(b4) plot the DOS on the ring for selected k_{\parallel} . These ρ_I are not symmetric relative to the scattering center since they are computed from the scattering wave function with a transmission slightly smaller than unity.

Figure 11(b3) (inner ring) displays a node in the center of the barrier, as expected for antibonding states. The ρ_I in Figs. 11(a3) and 11(b4), on the other hand, vary smoothly through the MgO barrier. We may conclude that the bonding combination of interface states causes the single ring in Fig. 11(a1) and the outer ring of Fig. 11(b1). The double



FIG. 13. (Color online) Layer-thickness dependence of the k_{\parallel} -resolved transmission probability of minority spins through Fe/MgO(*n*ML)/Fe(001) (n = 5,6,7) MTJs in the P configuration with clean interfaces for selected energies.

ring structure is evidence of the coexistence of two transport channels, i.e., the antibonding combination of low-energy and the bonding combination of high-energy interface states.

The explanation of the rings at E_1 and E_2 in Fig. 11 is supported by the energy dependence of the transmission probabilities in Fig. 12. There is only a single ring for $E - E_f \in (0.5, 0.92)$ eV, while a double ring structure is observed for $E - E_f \in (0.92, 1.1)$ eV, which is consistent with the double step feature in the energy-dependent conductance (black squares in the inset of Fig. 4).

The radius of the single ring increases with energy. However, at higher energy, the growth rate decreases and the double ring structure appears at $E = E_f + 0.92$ eV. The energy splitting between bonding and antibonding states in Table IV decreases with energy until the whole feature disappears.

Finally, the transmission probability in k_{\parallel} space as a function of MgO barrier thickness with specular interfaces (Fig. 13) reveals that the energy splitting of bonding and antibonding decreases with thicker MgO barriers, reflecting the reduced overlap between the two interface states. The maximum transmission does not change so the resonant tunneling is preserved for specular interfaces.

However, the resonant states are increasingly vulnerable to disorder scattering and decoherence, and their contribution to transport is expected to vanish in the thick-layer limit. We observe that the double ring feature vanishes for thick layers, indicating that the interaction of the higher-energy interface states is suppressed.

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