Exchange-driven spin Hall effect in anisotropic ferromagnets

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Crystallographic anisotropy of the spin-dependent conductivity tensor can be exploited to generate transverse spin-polarized current in a ferromagnetic film. This ferromagnetic spin Hall effect is analogous to the spin-splitting effect in altermagnets and does not require spin-orbit coupling. First-principles screening of 41 non-cubic ferromagnets revealed that many of them, when grown as a single crystal with tilted crystallographic axes, can exhibit large spin Hall angles comparable with the best available spin-orbit-driven spin Hall sources. Macroscopic spin Hall effect is possible for uniformly magnetized ferromagnetic films grown on some low-symmetry substrates with epitaxial relations that prevent cancellation of contributions from different orientation domains. Macroscopic response is also possible for any substrate if magnetocrystalline anisotropy is strong enough to lock the magnetization to the crystallographic axes in different orientation domains.

I. INTRODUCTION

The spin Hall effect [1, 2] is utilized for generating transverse spin currents which can be injected across interfaces into adjacent layers in heterostructures. If that spin current is injected into a magnetic layer, it can be converted into magnetization torque. For heavy-metal spin Hall layers, this is called spin-orbit torque [3] and is used as an alternative to spin-transfer torque for applications including magnetic random-access memory (MRAM), high-frequency oscillators, and neuromorphic computing [4, 5].

The spin Hall effect also exists in ferromagnets [6–18], where it has both time-reversal even and odd [18, 19] components. The odd component, referred to as the magnetic spin Hall effect, was also observed in noncollinear antiferromagnets [20–25]. The structure of the spin current response tensor in the presence of spin-orbit coupling may be deduced from the magnetic point group of the material [8]. Some magnets can exhibit spin Hall response even without spin-orbit coupling, in which case the symmetry of the response tensor may be determined using spin groups treating spatial and spin degrees of freedom separately from each other [26]. This was first noted for noncollinear antiferromagnets [20, 21].

Transverse spin currents without spin-orbit coupling are also possible [27–30] in so-called altermagnets [31, 32], i.e., collinear antiferromagnets with k-dependent exchange splitting allowed by symmetry. In this case, spin-orbit coupling usually plays a minor role and can be neglected, but the crystallographic orientation of the film is important. The exchange-driven spin Hall current in altermagnets has been referred to as the *spin-splitting current* [27–29]. For collinear two-sublattice antiferromagnets without spin-orbit coupling, the symmetry of the macroscopic response properties, including the spin Hall tensor, is fully described by the black-and-white (Heesch-Shubnikov) point group, while the polarization of the spin current is decoupled from the crystal axes and is simply parallel to the antiferromagnetic order parameter [33].

In contrast to the spin Hall effect in heavy metals, which is typically dominated by the intrinsic mechanism [2], the spin-splitting current in altermagnets scales with the longitudinal conductivity, leading to a disorder-independent spin Hall angle. This feature is shared with the magnetic spin Hall effect, which is also time-reversal-odd [18]. The predicted spin Hall angle for altermagnetic RuO_2 is about 0.27 [27], which compares favorably with spin-orbit-driven sources like Pt or β-W. However, observation of this large response may be hindered by the difficulty in achieving a single-domain state in RuO_2 due to the absence of uncompensated magnetization [29].

In this paper, I show that exchange-driven spin Hall effect can also be observed in ferromagnets and ferrimagnets thanks to the anisotropy of the spin-dependent conductivity tensor. As in the case of altermagnets, generation of the transverse spin current imposes restrictions on the bulk symmetry and the orientation of the film. In particular, the ferromagnet can not be cubic, and it needs to be grown such that the surface normal does not coincide with a principal axis of the conductivity tensor. Using first-principles calculations, I then estimate the spin Hall angles for a number of tetragonal, hexagonal, and orthorhombic ferromagnets and ferrimagnets, identifying a few with spin Hall angles as large as 0.3–0.4. Where possible, suitable substrates are suggested for growing films with the tilted high-symmetry axes, as required for the observation of the exchange-driven spin Hall current. If the film is uniformly magnetized, observation of the spin Hall current over a macroscopically large surface area requires that the bilayer has sufficiently low symmetry so that the spin Hall current is not cancelled out by averaging over degenerate orientation domains. These symmetry requirements may be fully relaxed if the ferromagnet has strong magnetocrystalline anisotropy which locks the magnetization to the crystallographic axes in different orientation domains.

The paper is organized as follows. Section II presents the analysis of the exchange-driven spin Hall response in a film with an anisotropic spin-dependent conductivity tensor. Section III describes computational details, and

the results are displayed in Section IV. Section V discusses crystallographic orientation domains and the statistical average of the spin Hall conductivity over these domains. The conclusions are summarized in Section VI.

II. TRANSVERSE SPIN CURRENT IN A MAGNETIC FILM WITH OPEN BOUNDARY CONDITIONS

Consider a metallic film with a collinear magnetization whose spin-dependent conductivity tensor is $\sigma^{\lambda}_{\alpha\beta}$, where the lower indices denote Cartesian components, and $\lambda \in \{\uparrow,\downarrow\}$ is the spin projection. I will also use $\lambda = \pm 1$ in equations. The conductivity tensor is symmetric because spin-orbit coupling is neglected, which imposes time-reversal invariance independently in each spin channel, and the spin projection is defined with respect to the orientation of the magnetic order parameter. Let the z axis point along the film normal direction and the x axis along the externally applied electric field E_x.

Because $\sigma^{\lambda}_{\alpha\beta}$ is anisotropic, the charge Hall response will generally lead to the build-up of Hall voltage across the thickness of the film. The resulting electric field component E_z is determined under the assumption of open-circuit boundary conditions, i.e., vanishing charge current density perpendicular to the film plane, $j_z = 0$. We then find the steady-state bulk spin current flowing perpendicular to the film plane. This spin current corresponds to the bulk spin Hall source term. To determine the spin current and accumulation profiles in a specific multilayer, this source term needs to be included in the spin-diffusion equations [34, 35]. A somewhat similar problem was considered for the transverse spin current driven by relativistic sources in a ferromagnetic film [9].

Explicitly, we have

$$j_x = \sum_{\lambda} \left[\sigma^{\lambda}_{xx} E_x + \sigma^{\lambda}_{xz} E_z\right] \tag{1}$$

$$j_z = \sum_{\lambda} \left[\sigma^{\lambda}_{zx} E_x + \sigma^{\lambda}_{zz} E_z\right] \tag{2}$$

$$j^s_z = \sum_{\lambda} \left[\sigma^{\lambda}_{zx} E_x + \sigma^{\lambda}_{zz} E_z\right] \lambda \tag{3}$$

where j^s_z is the spin current flowing in the z direction. Setting $j_z = 0$ and eliminating E_z, we find the effective spin Hall conductivity $\sigma_{\rm SH} = j^s_z/E_x$ and the effective longitudinal conductivity $\tilde{\sigma}_{xx} = j_x/E_x$ under open boundary conditions:

$$\sigma_{\rm SH} = \frac{\sigma_{zz}\sigma^s_{zx} - \sigma^s_{zz}\sigma_{zx}}{\sigma_{zz}} \tag{4}$$

$$\tilde{\sigma}_{xx} = \frac{\sigma_{xx}\sigma_{zz} - \sigma^2_{xz}}{\sigma_{zz}} \tag{5}$$

where $\sigma_{\alpha\beta} = \sum_\lambda \sigma^{\lambda}_{\alpha\beta}$ and $\sigma^s_{\alpha\beta} = \sum_\lambda \lambda\, \sigma^{\lambda}_{\alpha\beta}$. We are interested in the spin Hall angle under open boundary conditions defined as $\theta_{\rm SH} = \sigma_{\rm SH}/\tilde{\sigma}_{xx}$.

For the given crystallographic orientation of the film, the charge and spin conductivity tensors in Eqs. (4)-(5) may be expressed through their principal components. For simplicity, let us assume the principal axes of $\sigma_{\alpha\beta}$ and $\sigma^s_{\alpha\beta}$ are the same, which is true if they are fixed by symmetry; this is the case for tetragonal, hexagonal, and orthorhombic lattices considered below. Further, let us also assume that one of the principal axes is oriented in the plane of the film along the y axis. I denote the other two principal axes as 1 and 2 and the angle made by principal axis 1 with the z axis as θ. Applying the rotation by angle θ with respect to the y axis to the tensors expressed in their principal axes and substituting in Eqs. (4)-(5), we find, after some algebra:

$$\theta_{\rm SH} = \frac{1}{2}(\beta_1 - \beta_2)\sin 2\theta \tag{6}$$

where $\beta_i = \sigma^s_i/\sigma_i$ is the conventionally defined [35, 36] spin polarization of the conductivity along its principal axis i.

Equation (6) shows that $|\theta_{\rm SH}| \le 1$, and the maximal value of 1 is reached if $\theta = \pi/4$ and $\beta_1 = -\beta_2 = 1$. This maximal condition requires that the current along principal axes 1 and 2 is carried exclusively by spin-up and spin-down electrons, respectively, i.e., the ferromagnet behaves as a half-metal with opposite spin polarizations along the two principal axes. While this condition is unlikely to be satisfied by any material, we will see below that values of $|\theta_{\rm SH}|$ exceeding 0.1 are quite common, which compares favorably with the spin Hall angles typical of heavy metals such as Pt [2].

In the relaxation-time approximation [37], the conductivity tensor is given by

$$\sigma^{\lambda}_{\alpha\beta} = e^2 \sum_n \int v^{\lambda}_{n\alpha} v^{\lambda}_{n\beta} \tau^{\lambda}_n \frac{\partial f(E^{\lambda}_n)}{\partial \mu} \frac{d^3k}{(2\pi)^3} \tag{7}$$

where $\mathbf{v}^{\lambda}_n(\mathbf{k})$, $\tau^{\lambda}_n(\mathbf{k})$, and $E^{\lambda}_n(\mathbf{k})$ are the group velocity, relaxation time, and energy of the Bloch band n of spin λ, and $f(E)$ is the Fermi-Dirac distribution function at chemical potential μ for the given temperature. The relaxation-time approximation (7) is appropriate if disorder-induced broadening does not lead to significant overlap between electronic bands [38].

The relaxation times generally depend on the kind of impurities or other disorder present in the system, but, for a typical good metal with an extended Fermi surface and localized disorder that is typical for sputtered multilayers, it is reasonable to assume that $\tau^{\lambda}_n(\mathbf{k})$ depends only on spin λ. Then τ_λ can be pulled out of the integral in (7), and we have $\sigma^{\lambda}_{\alpha\beta} = e^2\tau_\lambda K^{\lambda}_{\alpha\beta}$, where the tensor $K^{\lambda}_{\alpha\beta}$ depends only on the electronic structure and can be calculated using standard techniques.

Introducing the spin polarizations of the relaxation time, $P_\tau = (\tau_\uparrow - \tau_\downarrow)/(\tau_\uparrow + \tau_\downarrow)$, and of the principal value i of tensor K, $P_i = (K^{\uparrow}_i - K^{\downarrow}_i)/(K^{\uparrow}_i + K^{\downarrow}_i)$, we find

$$\beta_i = \frac{P_\tau + P_i}{1 + P_\tau P_i} \tag{8}$$

and

$$\beta_1 - \beta_2 = \frac{(1-P_\tau^2)(P_1-P_2)}{(1+P_1P_\tau)(1+P_2P_\tau)}. \tag{9}$$

Equation (9) shows that the difference P_1-P_2, which is an easily calculable band structure property, can be used as a descriptor to screen for materials with large $|\beta_1-\beta_2|$. We should, however, bear in mind that this descriptor is only adequate as long as P_τ is not too large, in which case $|\beta_1-\beta_2|$ can be significantly reduced compared to $|P_1-P_2|$. On the other hand, if $P_1 \neq -P_2$, there is a range of P_τ of a certain sign that makes $|\beta_1-\beta_2|$ greater than $|P_1-P_2|$.

The (isotropic) transport spin polarization β in elemental ferromagnets Fe, Co, and Ni alloyed with a small amount of a second magnetic element varies drastically, including in sign, depending on the choice of that element [36, 39]. This suggests that magnetic impurities can be used to tune P_τ in a wide range as long as scattering is dominated by these impurities.

The spin polarization P of the isotropic tensor K in bcc Fe, fcc Co, and fcc Ni, calculated as described in Section III, is, respectively, 0.34, 0.05, and 0.02. The values for Co and Ni are small compared to the typical measured values of β in multilayer structures, such as 0.3–0.5 in Co or 0.5-0.8 in permalloy [36]. A theoretical calculation with explicit treatment of substitutional disorder in fcc $Ni_{1-x}Fe_x$ alloys resulted in β exceeding 0.5 in the whole compositional range [40]. This comparison suggests that β in these ferromagnets is often dominated by P_τ. However, in searching for materials with a large *anisotropy* of β, which, according to (6), is required for efficient transverse spin current generation, the anisotropy of P is of central importance, according to (9). Therefore, in the following I use the quantity $\tilde{\theta}_{ij} = \frac{1}{2}(P_i - P_j)$ as a proxy for the spin Hall angle of a film with geometry described before Eq. (6).

III. COMPUTATIONAL DETAILS

Using the Materials Project database [41], a set of experimentally reported ferro- and ferrimagnetic materials was selected using the following criteria: no more than three constituent elements, no rare earths (with the exception of GdNi) or actinides, metallic and magnetic DFT ground state, at least one $3d$ atom from V to Ni, with the tetragonal, hexagonal, or orthorhombic crystal structure. This set was further pruned, removing materials with no experimentally reported magnetic phase transition, in part using the database supplied with Ref. 42. Half-metallic, quasi-two-dimensional, and weakly ferromagnetic materials were also excluded, along with those with a large number of atoms per unit cell. The resulting set is by no means complete, but it provides a broad, representative selection.

The lattice structures were taken from the Materials Project database [41] and standardized using the `spglib` library [43] with a large tolerance of 0.5% to remove the occasional spurious symmetry reductions. The structures were then optimized using the projector-augmented wave (PAW) method [44], implemented in the Vienna Ab Initio Simulation Package (VASP) [45–47], using the generalized gradient approximation of Perdew-Burke-Ernzerhof (PBE) [48] for the exchange-correlation functional. The optimized lattice constants and magnetizations are listed in Table I.

For ferrimagnetic Mn_2Sb, it was found that the LDA+U method with $U = 2.0$ eV applied to the $3d$ shell of the Mn atoms in octahedral sites significantly improves agreement with experimental data ($a = 4.03$ Å, $c = 6.53$ Å, $M = 1.66$ μ_B/f.u.) [49] for the lattice constants and the magnetization. This calculation is labeled Mn_2Sb+U in Table I.

The tensor $K^\lambda_{\alpha\beta}$ was calculated using the smooth Fourier interpolation technique [51] implemented in the BoltzTrap2 package [52], which was slightly modified to obtain spin-resolved information. After structural optimization, the band eigenvalues were calculated on a Γ-centered k-point mesh with the distance between the mesh points in the direction of each reciprocal lattice vector set to approximately 0.1 $Å^{-1}$. The smooth Fourier interpolation included approximately 20 times more stars of real-space lattice vectors than irreducible k-points. It was checked that these parameters provided results for $\tilde{\theta}_{ij}$ converged to about 0.01.

IV. SPIN HALL ANGLES

Table II lists the calculated values of $\tilde{\theta}_{ij} = \frac{1}{2}(P_i - P_j)$ for selected materials. Note that $\tilde{\theta}_{xy} = 0$ by symmetry in tetragonal and hexagonal magnets.

Some of the largest values of $|\tilde{\theta}_{ij}|$ are found in $L1_0$-ordered MnGa (0.29), hexagonal MnSb (0.29), and orthorhombic FeB (0.37) and Mn_3Sn_2 (0.35). These values compare favorable with commonly used heavy-metal spin Hall sources, such as Pt and β-W [2, 3].

The last two columns of Table II include possible substrates, selected with the help of the Materials Project database [41], which can form a lattice-matched interface with the given material, and the corresponding minimal co-incident area (MCIA) [53] for that epitaxy. All of these epitaxial relations have the ferromagnetic film oriented so that there is no principal axis perpendicular to the film plane, thereby allowing spin Hall effect for a given orientation domain. Of course, there is no guarantee that these epitaxial relations can be realized in practice, and they should be regarded as illustrative examples.

TABLE I. Optimized (a, b, c) and experimental [50] ($a_{\rm exp}$, $b_{\rm exp}$, $c_{\rm exp}$) lattice constants (Å) and calculated magnetization M (μ_B/f.u.) for selected materials. Tetragonal, hexagonal, and orthorhombic magnets are separated by horizontal lines. MPID is the Materials Project identifier [41]. Mn_2Sb+U is Mn_2Sb treated with LDA+U (see text).

Material	MPID	a	b	c	$a_{\rm exp}$	$b_{\rm exp}$	$c_{\rm exp}$	M
FePt	mp-2260	2.723		3.764	2.729		3.713	3.28
FePd	mp-2831	2.708		3.770	2.722		3.714	3.29
CoPt	mp-949	2.690		3.715	2.691		3.684	2.27
MnAl	mp-771	2.755		3.476	2.772		3.57	2.32
MnGa	mp-1001836	2.705		3.660	2.748		3.676	2.51
FeNi	mp-2213	2.514		3.577	2.533		3.582	3.24
Fe_2B	mp-1915	5.046		4.228	5.11		4.249	3.67
Co_2B	mp-493	4.947		4.245	5.015		4.22	2.00
$MnAu_4$	mp-12565	6.520		4.045	6.45		4.04	4.16
VAu_4	mp-1069697	6.507		4.035	6.4		3.98	1.95
Mn_2Sb	mp-20664	3.921		6.419	4.085		6.534	1.28
Mn_2Sb+U	mp-20664	4.026		6.527	4.085		6.534	1.60
Fe_3B	mp-1181327	8.535		4.227	8.647		4.282	5.82
Fe_3P	mp-18708	9.042		4.374	9.107		4.460	5.68
Fe_8N	mp-555	5.681		6.223	5.718		6.288	19.3
Mn_2Ga_5	mp-607225	8.809		2.692	8.803		2.694	4.41
$Be_{12}Cr$	mp-1590	7.205		4.113	7.238		4.174	1.44
MnAlGe	mp-20757	3.882		5.922	3.89		5.925	2.02
Fe_5B_2P	mp-9913	5.441		10.31	5.477		10.345	8.52
CrTe	mp-794	4.128		6.273	4.005		6.242	3.88
MnBi	mp-568382	4.307		5.738	4.305		6.118	3.52
Fe_2P	mp-778	5.800		3.432	5.877		3.437	2.96
Fe_3N	mp-1804	4.652		4.317	4.708		4.388	6.17
YCo_5	mp-2827	4.912		3.941	4.951		3.975	7.03
MnAs	mp-610	3.665		5.498	3.710		5.691	2.90
MnSb	mp-786	4.094		5.602	4.12		5.79	3.19
$ZrFe_2$	mp-1190681	4.970		8.076	4.952		16.12	3.07
$HfFe_2$	mp-956096	4.944		8.027	4.968		8.098	3.05
Fe_3Ge	mp-21078	5.129		4.210	5.178		4.226	6.42
Fe_3Sn	mp-20883	5.468		4.302	5.458		4.361	6.99
YFe_3	mp-1192321	5.087		16.20	5.133		16.39	5.57
Fe_5Si_3	mp-449	6.697		4.677	6.541		4.558	7.62
Mn_5Ge_3	mp-617291	7.121		4.948	7.184		5.053	13.3
MnP	mp-2662	3.150	5.186	5.842	3.172	5.258	5.918	1.38
FeB	mp-20787	2.942	3.990	5.405	2.946	4.053	5.495	1.16
Mn_3Sn_2	mp-600428	5.398	7.457	8.420	5.510	7.565	8.598	7.74
Fe_3B	mp-973682	4.365	5.403	6.643	4.387	5.437	6.71	6.08
Fe_3C	mp-510623	4.478	5.033	6.722	4.512	5.082	6.742	5.58
Co_3B	mp-20373	4.396	5.145	6.603	4.418	5.232	6.636	3.53
Co_3C	mp-20925	4.426	4.93	6.686	4.483	5.033	6.731	3.05
GdNi	mp-542632	3.784	10.40	4.211	3.778	10.36	4.221	7.39
$AlFe_2B_2$	mp-3805	2.913	11.02	2.847	2.926	11.02	2.871	2.63

V. SPIN HALL DOMAINS

As will be discussed shortly below, many epitaxial relations allow more than one energetically degenerate orientation domain of the ferromagnetic film on the same substrate, characterized by different spin Hall conductivity tensors. In a large-area film, degenerate orientation domains should occur with equal probabilities, and macroscopic physical responses correspond to statistical averages over these domains. Of course, several nondegenerate interface terminations may coexist in one sample, resulting in more than one set of degenerate orientation domains occurring with different probabilities. This section discusses macroscopic spin Hall response of a multidomain ferromagnetic film from the symmetry point of view. If this response survives after statistical averaging over orientation domains, it can be observed either using macroscopic probes over length scales exceeding the orientation domain size or as an ensemble average over single-domain nanoscale devices where orientations domains occur at random.

I start with general considerations and then consider the case of uniform magnetization in Section V B, which imposes stringent symmetry requirements on the substrate and the epitaxial relation. Then Section V C turns to the case of strong magnetocrystalline anisotropy,

TABLE II. Spin polarizations P_i of the principal values of tensor $K^{\lambda}_{\alpha\beta}$ and maximal exchange-driven spin Hall angles $\tilde{\theta}_{ij}$ calculated assuming $P_\tau = 0$ and $\theta = \pi/4$ for selected magnetic materials. T_c (K) is the experimental Curie temperature. Substrate/Magnet: a possible substrate, obtained using the Materials Project [41], and its epitaxial relation, such that the interface normal of the magnetic material is not oriented along any of the principal axes of its $K^{\lambda}_{\alpha\beta}$ tensor. MCIA: minimal co-incident area (Å^2) for that epitaxy [53]. G_{sub}: crystallographic point group of the substrate. G_{bil} (listed when $G_{sub} = C_{1v}$): crystallographic point group of the bilayer. Substrates allowing a finite macroscopic spin Hall effect for a uniformly magnetized ferromagnetic film ($G_{sub} = C_1$ or $G_{sub} = G_{bil} = C_{1v}$) are highlighted in bold. All cases with $G_{sub} = C_{1v}$ and $G_{bil} = C_1$ belong to case (3) of Sec. V B. a-TiO_2 stands for anatase and TiO_2 for rutile.

Material	T_c	P_x	P_y	P_z	$\tilde{\theta}_{zx}$	$\tilde{\theta}_{zy}$	$\tilde{\theta}_{xy}$	Substrate/Magnet	MCIA	G_{sub}	G_{bil}
FePt	753	0.34		0.24	−0.05		0	**$NdGaO_3$ (011)/(101)**	51	C_{1v}	C_{1v}
FePd	1193	0.37		0.31	−0.03		0	**$NdGaO_3$ (011)/(101)**	51	C_{1v}	C_{1v}
CoPt	846	0.23		0.07	−0.08		0	**$YAlO_3$ (011)/(101)**	51	C_{1v}	C_{1v}
MnAl	650	0.05		0.55	0.25		0	**$NdGaO_3$ (011)/(101)**	49	C_{1v}	C_{1v}
MnGa	629	0.07		0.64	0.29		0	**$NdGaO_3$ (011)/(101)**	49	C_{1v}	C_{1v}
FeNi	842	0.27		0.36	0.04		0	h-BN (0001)/(101)	11	C_{6v}	
Fe_2B	1013	0.37		0.06	−0.16		0	$LiGaO_2$ (010)/(101)	33	C_{1v}	C_1
Co_2B	433	0.34		0.63	0.14		0	$LiGaO_2$ (010)/(101)	32	C_{1v}	C_1
$MnAu_4$	385	0.45		0.49	0.02		0	GaSe (0001)/(101)	51	C_{6v}	
VAu_4	60	−0.54		−0.58	−0.02		0				
Mn_2Sb	580	0.50		0.15	−0.17		0	MgF_2 (101)/(111)	78	C_{1v}	C_1
Mn_2Sb+U	580	0.35		−0.09	−0.22		0	MgF_2 (101)/(111)	78	C_{1v}	C_1
Fe_3B	828	0.47		0.70	0.12		0				
Fe_3P	693	0.70		0.77	0.03		0	Fe_2O_3 (0001)/(101)	91	C_{3v}	
Fe_8N	1500	0.03		0.26	0.12		0	$BaTiO_3$ (110)/(101)	48	C_{1v}	C_1
Mn_2Ga_5	450	0.47		0.20	−0.14		0	TiO_2 (100)/(101)	83	C_{2v}	
$Be_{12}Cr$	50	−0.13		−0.54	−0.21		0				
MnAlGe	520	0.42		0.88	0.23		0	**a-TiO_2 (101)/(101)**	83	C_{1v}	C_{1v}
Fe_5B_2P	628	0.23		0.17	−0.03		0	$GdScO_3$ (001)/(101)	64	C_{2v}	
CrTe	340	0.30		0.68	0.19		0	$LiAlO_2$ (110)/(10$\bar{1}$1)	90	C_2	
MnBi	633	0.86		0.42	−0.22		0	o-WTe_2 (001)/(10$\bar{1}$1)	89	C_{2v}	
Fe_2P	217	0.28		0.43	0.07		0	LiF (110)/(10$\bar{1}$1)	71	C_{2v}	
Fe_3N	858	−0.14		−0.01	0.07		0	C (0001)/(11$\bar{2}$1)	79	C_{6v}	
YCo_5	980	0.51		0.63	0.06		0	GaN (10$\bar{1}$1)/(10$\bar{1}$1)	57	C_{1v}	C_1
MnAs	318	0.75		0.29	−0.23		0	GaN (10$\bar{1}$1)/(10$\bar{1}$1)	116	C_{1v}	C_1
MnSb	851	0.91		0.33	−0.29		0	MgF_2 (110)/(10$\bar{1}$1)	82	C_{2v}	
$ZrFe_2$	630	−0.38		−0.41	−0.02		0				
$HfFe_2$	600	−0.26		−0.05	0.10		0	MgO (100)/(11$\bar{2}$1)	72	C_{4v}	
Fe_3Ge	670	0.16		0.46	0.15		0	Cu(100)/(10$\bar{1}$1)	94	C_{4v}	
Fe_3Sn	748	0.72		0.52	−0.10		0	$LaAlO_3$ (10$\bar{1}$0)/(10$\bar{1}$1)	70	C_{1v}	C_1
YFe_3	552	−0.08		0.21	0.15		0				
Fe_5Si_3	383	0.51		0.20	−0.15		0	GaAs (100)/(11$\bar{2}$1)	67	C_{2v}	
Mn_5Ge_3	296	0.54		0.66	0.06		0	BaF_2 (100)/(11$\bar{2}$1)	76	C_{4v}	
MnP	293	0.27	−0.23	0.24	−0.01	0.24	0.25	MgO (100)/(110)	36	C_{4v}	
FeB	598	−0.53	−0.36	0.21	0.37	0.28	−0.09	**SiO_2 (10$\bar{1}$0)/(110)**	27	C_1	
Mn_3Sn_2	262	−0.25	0.44	0.27	0.26	−0.09	−0.35	CaF_2 (100)/(011)	61	C_{4v}	
Fe_3B	828	0.66	0.40	0.69	0.02	0.14	0.13	MgO (100)/(011)	37	C_{4v}	
Fe_3C	480	0.25	−0.01	0.46	0.11	0.24	0.13	**SiO_2 (10$\bar{1}$0)/(101)**	81	C_1	
Co_3B	747	0.66	0.52	0.73	0.04	0.11	0.07	**ZrO_2 (101)/(101)**	41	C_{1v}	C_{1v}
Co_3C	498	0.38	0.38	0.49	0.05	0.06	0.00	**SiO_2 (10$\bar{1}$0)/(101)**	79	C_1	
GdNi	78	0.10	−0.11	−0.19	−0.14	−0.04	0.10	$BaTiO_3$ (111)/(101)	58	C_{1v}	C_1
$AlFe_2B_2$	285	0.73	0.55	0.73	0.00	0.09	0.09	CdS (0001)/(111)	46	C_{6v}	

which enables macroscopic spin Hall response even for high-symmetry substrates.

A. General considerations

Let G_{sub} and $G_{\rm FM}$ be the (nonmagnetic) surface point groups of the substrate alone and the ferromagnetic layer alone, respectively, and G_{bil} the point group of the epitaxial bilayer. G_{bil} is a common subgroup of G_{sub} and $G_{\rm FM}$, and I assume $G_{bil} = G_{sub} \cap G_{\rm FM}$ when viewed as a set. Of course, G_{bil} depends on the mutual orientation of the symmetry elements of G_{sub} and $G_{\rm FM}$.

Neglecting the non-symmorphic components of the symmetry operations automatically incorporates statistical averaging over interface roughness [54]. This is the

reason to consider point groups rather than space groups.

Because the ferromagnetic layer is assumed to have tilted principal axes of the conductivity tensor, we require that $G_{\rm FM}$ is at most C_{1v}, which implies that G_{bil} is also at most C_{1v}.

If G_{bil} is a *proper* subgroup of G_{sub}, the same substrate supports several energetically degenerate crystallographic orientations of the ferromagnetic layer grown on top of that substrate. The set of these degenerate orientations is analogous to the orientation states of a ferroic crystal [55]. Different orientation domains are mapped onto each other by the symmetry operations in G_{sub}. The number of inequivalent orientation domains is equal to the index of G_{bil} in G_{sub} (see Theorem 3 of Ref. [55]), and they can be classified by the left cosets of G_{bil} in G_{sub}.

B. Uniform magnetization

Here I discuss statistical averaging of the spin Hall conductivity over one set of degenerate orientation domains that are all magnetized in the same direction, allowing the spin degree of freedom to be treated as a scalar quantity. This case is realized when the magnetocrystalline anisotropy is weak, and the entire film is uniformly magnetized by an application of an external magnetic field.

In the most general case, the effective longitudinal conductivities (5) and the effective Hall conductivities of different orientation domains from the same degenerate set may be different, leading to an inhomogeneous current density and electric field distribution. The inhomogeneity of the electric field over different orientation domains can, in principle, lead to a finite spin Hall response even if the average spin Hall conductivity vanishes. I will disregard this possibility and assume that the effective charge conductivity is approximately isotropic.

Generalizing Eq. (4) to an arbitrary direction of the in-plane electric field, the spin Hall current flowing perpendicular to the film can be written as $j^s_z = \mathbf{p}_{\rm SH}\mathbf{E}$, where $(\mathbf{p}_{\rm SH})_\alpha = \sigma^s_{z\alpha} - \sigma^{-1}_{zz}\sigma^s_{zz}\sigma_{z\alpha}$ and $\alpha \in \{x, y\}$. The in-plane polar vector $\mathbf{p}_{\rm SH}$ describes the out-of-plane spin Hall current of a given orientation domain and is invariant under $G_{\rm FM}$. In the case considered in the derivation of Eq. (6), when one principal axis of $\hat{\sigma}^\lambda$ lies in the plane, $\mathbf{p}_{\rm SH}$ is perpendicular to that axis.

The star of vectors $\mathbf{p}^{(i)}_{\rm SH}$ describing different orientation domains i belonging to the same degenerate set is generated by the symmetry operations from G_{sub}. The macroscopic spin Hall response is given by an average over this star. For it to be finite, it is necessary that G_{sub} allows an in-plane polar vector, which is only the case for $G_{sub} = C_1$ or C_{1v}. For $G_{sub} = C_1$ there is only one orientation domain, and it is sufficient that $\mathbf{p}_{\rm SH} \neq 0$ for it.

For $G_{sub} = C_{1v}$, let σ_v be the mirror plane of the G_{sub} group. There are three possibilities:

1. $G_{bil} = G_{sub} = C_{1v}$. There is only one orientation domain because G_{bil} is not a proper subgroup of G_{sub}. Because we have already assumed that $G_{\rm FM}$ is at most C_{1v}, and $G_{bil} = C_{1v}$ is its subgroup, it must be that $G_{\rm FM} = G_{\rm sub}$ with the same σ_v. Therefore, $\mathbf{p}_{\rm SH} \parallel \sigma_v$ and finite.

2. $G_{bil} = C_1$ and $\mathbf{p}_{\rm SH}$ has a finite projection on σ_v. This means that either $G_{\rm FM} = C_1$ or $G_{\rm FM} = C_{1v}$ but its symmetry plane is not orthogonal to σ_v of G_{sub}. There are two orientation domains but $\mathbf{p}^{(1)}_{\rm SH} + \mathbf{p}^{(2)}_{\rm SH} \neq 0$, and the microscopic average is finite.

3. $G_{bil} = C_1$ and $\mathbf{p}_{\rm SH} \perp \sigma_v$. This happens if $G_{\rm FM} = C_{1v}$ with the symmetry plane orthogonal to σ_v of G_{sub}. There are two orientation domains with $\mathbf{p}^{(1)}_{\rm SH} = -\mathbf{p}^{(2)}_{\rm SH}$, and the microscopic average vanishes.

Thus, a finite macroscopic spin Hall current is allowed for $G_{sub} = C_1$ and only in cases (1) and (2) for $G_{sub} = C_{1v}$. To maximize this current, the electric field should be aligned parallel to the average of $\mathbf{p}^{(i)}_{\rm SH}$ over the orientation domains.

1. *Substrate examples*

The point groups G_{sub} are listed in Table II for all substrates. Many of them are higher than C_{1v}, which guarantees that the macroscopic spin Hall conductivity vanishes after averaging over uniformly magnetized degenerate orientation domains.

A generic orientation of the surface plane would result in $G_{sub} = C_1$ for any crystalline substrate and allow macroscopic spin Hall effect, but this case is uncommon for readily available substrates. In Table II it is realized by SiO_2 $(10\bar{1}0)$, which may be matched with orthorhombic FeB (110), Fe_3C (101), or Co_3C (101). The D_3 bulk point group of SiO_2 has no mirror planes, and the $(10\bar{1}0)$ plane (also known as the Y-cut) is not orthogonal to a symmetry axis.

For substrates with $G_{sub} = C_{1v}$, we need to distinguish among the three cases listed above, and Table II also includes G_{bil}. Substrates corresponding to Case (1), which allows macroscopic spin Hall effect, have $G_{sub} = G_{bil} = C_{1v}$ and are highlighted in bold in Table II. The largest values of $\tilde{\theta}_{\alpha\beta}$ estimated for these systems are in $L1_0$-ordered MnAl (101) and MnGa (101) on $NdGaO_3$ (011) and for MnAlGe (101) on anatase TiO_2 (101) [56]. Note that the $L1_0$-ordered τ-phase of MnAl is metastable but can be stabilized by allowing with Ga [57]. $NdGaO_3$ (011) and $YAlO_3$ (011) substrates [58] present an interesting case where the C_{3v} point group of the (111) surface of the parent perovskite structure is broken by the bulk orthorhombic distortion, resulting in $G_{sub} = C_{1v}$.

Case (2) for $G_{sub} = C_{1v}$ requires that the symmetry planes of the substrate and the ferromagnet are neither

parallel nor orthogonal to each other. I have not found examples of this case.

Case (3) for $G_{sub} = C_{1v}$, which results in zero macroscopic spin Hall conductivity, is rather common and is realized, for example, in (101)-oriented FePt or MnGa grown on rutile TiO_2 (101) and in all other cases in Table II with $G_{sub} = C_{1v}$ that are not highlighted.

C. Case of strong magnetocrystalline anisotropy

In this case, the magnetizations in different orientation domains are generally not collinear with each other. As I show below, this allows one to obtain a finite macroscopically averaged spin Hall current even if G_{sub} includes a high-order symmetry axis, and the spin polarization of that current can be switched both in sign and in orientation by changing the direction of the initializing external magnetic field and the direction of the current flow.

Because there is no longer a globally defined direction of magnetization, we need to restore the vector character of the spin polarization when averaging over the orientation domains. I will assume that the magnetization is uniform inside each orientation domain, which is reasonable if the domain size is large compared to the magnetic domain wall width. The out-of-plane spin current for orientation domain i can be written as $\mathbf{j}_s^{(i)} = \hat{\mathbf{m}}^{(i)}(\mathbf{p}_{\rm SH}^{(i)} \cdot \mathbf{E})$, where the unit vector $\hat{\mathbf{m}}^{(i)}$ denotes the direction of the magnetization in orientation domain i. The subscript z for the direction of spin current flow has been omitted but is implied throughout. The macroscopic average of the 3×2 spin conductivity tensor is given by the tensor $\hat{\sigma}_{\rm SH} = \sum_i \hat{\mathbf{m}}^{(i)} \otimes \mathbf{p}_{\rm SH}^{(i)}/N_i$, where N_i is the number of orientation domains.

To be specific, let us consider the case of dominant bulk easy-axis anisotropy in a tetragonal or hexagonal ferromagnet with $G_{\rm FM} = C_{1v}$. In this case the magnetization lies in the plane containing the surface normal and the bulk fourfold or sixfold (or threefold) axis, which, as above, is tilted by angle θ with respect to the z axis. The angle made by $\hat{\mathbf{m}}^{(i)}$ with the z axis will be denoted as θ_m, which may differ from θ due to the demagnetizing field but is the same for all i, at least once the external field has been switched off.

Along with the $\mathbf{p}_{\rm SH}^{(i)}$ vector, the operations in G_{sub} also transform the orientation of the easy magnetization axis while keeping θ unchanged. First, assume the sample is magnetized by an out-of-plane magnetic field $\mathbf{B} = B_z\hat{z}$, so that $m_z^{(i)}$ is the same in all orientation domains. Because $m_z^{(i)}$ behaves as a scalar under G_{sub}, the z-polarized spin current behaves exactly as described in Section V B for the case of uniform magnetization.

On the other hand, the in-plane projection $\mathbf{m}_\parallel^{(i)}$ transforms like a polar vector under G_{sub}, similar to $\mathbf{p}_{\rm SH}^{(i)}$. (That $\mathbf{m}_\parallel^{(i)}$ formally behaves here as a polar rather than axial vector is enforced by the external field which selects the same sign of $m_z^{(i)}$ for all orientation domains.) Our assumption of $G_{\rm FM} = C_{1v}$ leads to $\mathbf{m}_\parallel^{(i)} \parallel \mathbf{p}_{\rm SH}^{(i)}$. Thus, the spin Hall conductivity $\hat{\sigma}_{\rm SH}^\parallel$ giving the out-of-plane flow of in-plane-polarized spins is equal to the average of $\pm p_{\rm SH}\, \hat{p}_{\rm SH}^{(i)} \otimes \hat{p}_{\rm SH}^{(i)} \sin\theta_m$ over all orientation domains, where $\hat{p}_{\rm SH}^{(i)} = \mathbf{p}_{\rm SH}^{(i)}/p_{\rm SH}$ and the overall sign is that of $\mathbf{m}_\parallel^{(i)} \cdot \mathbf{p}_{\rm SH}^{(i)}$, which in turn depends on the sign of B_z. The average over i survives under *any* point group G_{sub}. If G_{sub} includes a threefold or higher rotation axis, $\hat{\sigma}_{\rm SH}^\parallel$ reduces to a scalar $\sigma_{\rm SH}^\parallel = \pm\frac{1}{2} p_{\rm SH} \sin\theta_m$. Thus, we find an interesting situation where the spin polarization of the macroscopically averaged spin current flowing in the z direction is locked parallel to the direction of the in-plane charge current flow. This is in contrast to the conventional spin-orbit-driven spin Hall effect in nonmagnetic materials where the spin current would be polarized perpendicular to the current flow direction.

The situation is more complicated if the system is initialized by an in-plane magnetic field $\mathbf{B}$, rather than out-of-plane as above. The spin Hall current depends on G_{sub}, on the orientation of the initializing magnetic field, and on the orientation of the charge current flow, with respect to the symmetry elements of G_{sub} and $G_{\rm FM}$. For example, consider $G_{sub} = C_{4v}$ and $G_{\rm FM} = C_{1v}$, and align the x axis parallel to the coincident mirror planes of G_{sub} and $G_{\rm FM}$ for one of the orientation domains. There are four orientation domains with $\mathbf{p}_{\rm SH}^{(i)}$ oriented along the positive and negative directions of the x and y axes. For each domain, it is assumed the magnetization picks one of the two directions along its easy axis such that $\mathbf{m}^{(i)}\mathbf{B} > 0$. Then the averaged spin Hall current is strictly z-polarized: $\mathbf{j}_s = \frac{1}{2}\hat{z}\, p_{\rm SH} \cos\theta_m (\pm 1, \pm 1) \cdot \mathbf{E}$, where the signs for the vector components in brackets are such that this vector lies in the same quadrant with $\mathbf{B}$.

Another interesting example is when $\mathbf{B}$ is applied in the x direction with a small tilt toward z. In this case, the average spin Hall current is $\mathbf{j}_s = \frac{1}{2} p_{\rm SH}(0, E_y \sin\theta_m, E_x \cos\theta_m)$, and its polarization can be switched between in-plane and out-of-plane by changing the direction of the current flow.

As a function of the orientation of the initializing magnetic field $\mathbf{B}$, the spin Hall conductivity tensor has discontinuities along the contours on the sphere where one or more orientation domains switch their magnetization. After initialization, the measurement may be performed in the remanent state.

VI. SUMMARY

A crystalline ferromagnetic (or ferrimagnetic) film with tilted principal axes of the conductivity tensor can exhibit exchange-driven spin Hall effect, generating spin-polarized current perpendicular to the film surface, thanks to the anisotropy of the conductivity tensor. This

effect is analogous to the spin-splitting current in altermagnets and does not require spin-orbit coupling. First-principles screening of 41 tetragonal, hexagonal, and orthorhombic ferromagnets revealed that, for certain crystallographic orientations, the spin Hall angle is greater than 0.1 in 26 of them, and greater than 0.2 in 12.

To allow the use of this exchange-driven spin Hall effect on a macroscopic scale, the response should not vanish after averaging over the crystallographic orientation domains of the ferromagnetic film. For a uniformly magnetized sample, this is possible only if the substrate has low enough symmetry (C_1 or C_{1v}); moreover, for a C_{1v} substrate, the ferromagnetic film should not be aligned in such a way that two degenerate orientation domains have opposite spin Hall angles. If these conditions are not met, the macroscopic spin Hall conductivity of a uniformly magnetized film vanishes after averaging over degenerate orientation domains. Several cases listed in Table II do meet these conditions, most notably MnAl (101) and MnGa (101) on $NdGaO_3$ (011) and MnAlGe (101) on anatase TiO_2 (101), with rather large estimated spin Hall angles. In all systems listed in Table II the spin Hall effect may be observed locally for each orientation domain, for example, with a spatially resolved measurement of the magneto-optic Kerr effect.

The spin Hall effect can also be observed on the macroscopic scale, *regardless* of the substrate symmetry, if the ferromagnetic film has magnetocrystalling anisotropy strong enough to lock the magnetization to the crystallographic easy axis in each orientation domain. Multiple possibilities exist depending on the crystallographic symmetry and the orientation of the initializing magnetic field, including the averaged spin Hall current being polarized parallel to the current flow or perpendicular to the film plane.

Exchange-driven spin Hall effect in ferromagnets expands the range of available spin Hall sources for applications in magnetic heterostructures. In particular, one can envision a trilayer heterostructure in which the ferromagnetic source layer is separated from the detector layer by a nonmagnetic spacer, such as Cu, which is sufficiently thick to eliminate the exchange coupling between the layers. If the source ferromagnet has strong magnetocrystalline anisotropy, the spin Hall current can have a large out-of-plane component, facilitating the switching of the detector layer with perpendicular magnetization; this opportunity is advantageous for applications in magnetic random-access memory. In contrast to an altermagnet, the source ferromagnetic layer can be deterministically initialized by an external magnetic field. In terms of its device structure, the ferromagnetic trilayer spin Hall device is similar to a spin-orbit torque bilayer [3], where, in contrast with spin-transfer torque devices, the read and write current paths are separated.

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