Magnetization direction dependent spin Hall effect in 3d ferromagnets

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We have studied the intrinsic spin Hall conductivity in 3d transition metal ferromagnets using first principle calculations. We find the spin Hall conductivity of bcc-Fe and fcc-Ni, prototypes of ferromagnetic systems, depends on the direction of magnetization. The spin Hall conductivity of electrons with their spin orientation orthogonal to the magnetization are found to be larger than that when the two are parallel. For example, the former can be more than four times larger than the latter in bcc-Fe. Such difference arises due to the anisotropy of the spin current operator in the spinor space: its expectation value with the Bloch states depends on relative angle between the conduction electron spin and the magnetization. These results show that ferromagnets can be used to generate spin current and its magnitude can be controlled by the magnetization direction.

INTRODUCTION

The spin Hall effect (SHE) allows generation of spin current when current is passed to materials with large spin orbit coupling (SOC). Such spin current can be used to manipulate the magnetization direction of a nearby ferromagnet using the spin transfer torque, or the so-called spin orbit torque. Giant spin Hall effect has been found in non-magnetic 5d transition metals. Search for materials with large spin Hall effect has been expanded into various systems, including ferromagnets and antiferromagnets.

Model calculations have predicted that ferromagnets can be used to generate spin accumulation through its anomalous Hall effect (AHE). Experimentally it has been shown that the spin accumulation from the AHE in ferromagnets can be used to manipulate the magnetic moments of a nearby ferromagnetic or ferrimagnetic layer. Under such circumstance, the degree of spin accumulation from the AHE can be tuned by the magnetization direction of the ferromagnetic layer. The spin Hall effect in ferromagnets, in contrast, is not well understood partly because of the difficulty in distinguishing spin current from the AHE and SHE. Recent experiments indicate contradictory pictures on the SHE in ferromagnets, suggesting that it can either be dependent or independent of the magnetization direction. The underlying physics of SHE in ferromagnets thus remains to be identified.

With the emergence of topology in condensed matter physics, the AHE has been reformulated in the language of geometric phase, i.e. the Berry phase. Intrinsic contribution of the anomalous Hall conductivity (AHC) can be calculated through Kubo formula in its spectral representation, which is mathematically identical to the Berry phase representation. In analogy to AHC, intrinsic contribution of the spin Hall conductivity (SHC) can be also calculated using the Kubo formula by replacing the electron velocity operator with a spin current velocity operator. In this context, it is widely accepted that the SHE and AHE share the same theoretical framework.

In this paper, we study the SHE of ferromagnets using first principle calculations with the generalized Kubo formula. We use bcc-Fe and fcc-Ni as prototypes of the ferromagnetic system. One of the key features in ferromagnets is the existence of large exchange interaction, which breaks the SU(2) rotation symmetry in the spinor space. We release the constraint of parallel configuration between the spontaneous magnetization and the spin quantization axis of the conduction electrons. We find the magnitude of the intrinsic spin Hall conductivity (SHC) in Fe and Ni can be varied via changes in the magnetization direction with respect to the spin polarization of the conduction electrons. The spin Berry curvature and the Berry curvature are mapped in the momentum space together with the spin character of the corresponding bands to study their correlation.

CALCULATION MODEL

The density functional theory (DFT) calculations is performed by full-potential linearized augmented-plane-wave method with generalized gradient approximation for the exchange correlation. The primitive cell of bcc-Fe and fcc-Ni are constructed with lattice constant chosen from experimentally determined values, \( a_{\text{Fe}} = 2.86\AA, a_{\text{Ni}} = 3.52\AA \). Muffin-tin (MT) radius are taken 2.2 bohrs for both Fe and Ni, respectively. The angular momentum expansion inside MT spheres is truncated at \( l = 8 \) for the wave functions, charge and spin densities, and potential. The reciprocal \((k-)\) space is divided into \( 16 \times 16 \times 16 \) meshes for calculating charge and spin densities. The spin orbit coupling is treated via the second variational method.
The Bloch states are represented by a linear combination of the LAPW basis functions multiplied with a spinor

$$\Psi_{k,n}(r) = \sum_{q=k+G} G_{\text{max}} C_{q,n} \psi_{q,n}(r) \chi_{q,n}. \quad (1)$$

$\psi_{q,n}(r)$ is the LAPW basis function, $\chi_{q,n}$ is the two component spinor that represents the spin direction of the state $(q,n)$, and $C_{q,n}$ is the expansion coefficient. $G$ is the reciprocal lattice vector. LAPW functions have a cutoff: $G_{\text{max}}$ is the cutoff vector with $|G_{\text{max}}| = 3.9$ a.u.$^{-1}$. The electron density

$$\rho_\alpha(r) = \sum_k \sum_{n \in \text{occ}} \Psi_{k,n}^\dagger(r) \sigma_\alpha \Psi_{k,n}(r) \quad (2)$$

contains a $U(1)$ part and a $SU(2)$ part, i.e. $\rho_\alpha(r) = (\rho_\alpha(r), m_\alpha(r))$, where $\rho_\alpha(r)$ and $m_\alpha(r)$ correspond to charge density and spin density, respectively. $\sigma_\alpha$ represents the generalized Pauli matrix which has four components in our convention, $\sigma_\alpha = (I_2, \sigma_\alpha)$. $I_2$ is a $2 \times 2$ unit matrix, $\sigma_\alpha$ is the Pauli matrix, the greek indices (e.g. $\alpha, \beta$) run from 0 to 3 representing four vectors, and the roman indices (e.g. $i,j,k$) correspond to space coordinates (i.e. $x,y,z$).

The Kohn-Sham single-particle Hamiltonian is written as

$$\mathcal{H} = \mathcal{H}_{\text{kin}} I_2 + V_\alpha(r) \sigma_\alpha. \quad (3)$$

$\mathcal{H}_{\text{kin}}$ is kinetic energy term and $V_\alpha = (V_0(r), V_\beta(r))$ is the effective potential with a non-magnetic $U(1)$ part and a magnetic $SU(2)$ part. In our calculation, the spin quantization axis is fixed along the $z$-axis in the Cartesian coordinate. Computations are carried out for two different magnetic configurations, noted as $m_z$ and $m_x$, by setting the magnetic moment along $z$ and $x$, respectively. Bcc-Fe and fcc-Ni are chosen as prototypes of ferromagnets which do not exhibit significant crystalline anisotropy.

The intrinsic anomalous Hall conductivity (AHC) and the intrinsic spin Hall conductivity (SHC) are obtained from the linear response Kubo formula in the static limit.[13, 14, 25, 28] We define the off-diagonal conductivity tensor $\sigma^{ij}_{\alpha}$ as

$$\sigma^{ij}_{\alpha} = -e^2 \hbar \int_{BZ} \frac{d^3k}{(2\pi)^3} \Omega^{ij}_{\alpha}(\mathbf{k}) \quad (4)$$

$$\Omega^{ij}_{\alpha}(\mathbf{k}) = -\sum_{n' \neq n} \left[ f(\epsilon_n(\mathbf{k})) - f(\epsilon_{n'}(\mathbf{k})) \right] \times \text{Im} \left[ \langle \mathbf{k}, n| \hat{v}^\alpha_{\mathbf{i}} | \mathbf{k}, n' \rangle \langle \mathbf{k}, n'| \hat{v}^0_{\mathbf{j}} | \mathbf{k}, n \rangle \right] \left( \epsilon_n(\mathbf{k}) - \epsilon_{n'}(\mathbf{k}) \right)^2 \quad (5)$$

where $\Omega^{ij}_{\alpha}$ represents the generalized Berry curvature. $v^0_{ij} = \frac{1}{2} \{\sigma, v_j\}$ is the general velocity operator with the subscript and superscript denoting the spatial coordinate and the spin quantization axis[29], respectively. $v_i$ and $v^k_i$ are the charge velocity and spin velocity operator, $\Omega^{ij}_{\alpha}$ and $\Omega^{ij}_{\alpha}$ are the Berry and spin Berry curvatures, and $\sigma^{ij}_{\alpha}$ and $\sigma_{\alpha}$ are the AHC and SHC, respectively. With the zero-temperature assumption employed in our calculations, the Fermi distribution $f(\epsilon(\mathbf{k}))$ reduces to a step function $\Theta(\epsilon_F - \epsilon(\mathbf{k}))$ ($\epsilon_F$ is the Fermi energy). To reduce numerical error, we extend the size of $k$-point mesh up to $64 \times 64 \times 64$ with total of 262,144 special $k$ points inside the first BZ to calculate the SHC.

**RESULTS AND DISCUSSIONS**

The AHC and SHC for the two magnetization configurations are presented in Table. I. The values of the intrinsic AHC of bcc-Fe and fcc-Ni show good agreement with previous reports.[13, 30]

| Sample    | $\sigma_{yx}^0$ | $\sigma_{yx}^0$ | $\sigma_{yx}^0$ | $\sigma_{yx}^0$ | $m_{\text{tot}}$ |
|-----------|----------------|----------------|----------------|----------------|-----------------|
| bcc-Fe ($m_z$) | 747 | 0 | 130 | 0 | 2.18 |
| bcc-Fe ($m_x$) | 0 | 747 | 527 | 0 | 2.18 |
| fcc-Ni ($m_z$) | -2414 | 0 | 1535 | 0 | 0.60 |
| fcc-Ni ($m_x$) | 0 | -2414 | 2358 | 0 | 0.60 |
FIG. 2. (a-h) Berry and spin Berry curvatures projected on first Brillouin zone with two different magnetic configurations. The left and right panels present results when the magnetization points along $z$ and $x$, respectively. (a-d) show calculation results for bcc-Fe, (e-h) display those for fcc-Ni. (a,e) $\Omega^0_{yx}$, (b,f) $\Omega^0_{zy}$, (c,d,g,h) $\Omega^3_{yx}$.

For both bcc-Fe and fcc-Ni, the non-vanishing component of the AHC changes from $\sigma^0_{yx}$ to $\sigma^0_{zy}$ when the magnetization direction is changed from along the z axis to x axis. The magnitude of the non-vanishing component of the AHC remains the same. We have also studied the total magnetic moment of the system, which are found to be identical for both magnetic configurations. These results are consistent with the symmetry of cubic systems. In contrast, the non-vanishing component of SHC, $\sigma^3_{yx}$, does not change when the magnetization direction is changed. Note that here we have chosen the z axis as the spin quantization axis[31]: thus spin current with polarization along the z axis is studied. (One may chose the spin quantization axis to follow the magnetization direction, as is done for most cases; however, the SHC will be invariant for cubic systems under such circumstance.) Interestingly, the magnitude of SHC varies drastically with changes in the magnetization direction. For example, in bcc-Fe, the SHC changes from 130 S/cm to 520 S/cm when the magnetization direction is rotated from z to x. Such magnetization direction dependent SHC in ferromagnets is the main findings of this paper.

To analyze the change in SHC with respect to the magnetization direction ($m_z$ and $m_x$), we first show stereoscopic mapping of the non-vanishing components of the Berry curvature ($\Omega^0_{yx}$) and the spin Berry curvature ($\Omega^3_{yx}$) projected in the first Brillouin zone. For bcc-Fe, upon rotating the magnetization from $z$ to $x$, the Berry curvature rotates following the the profile of the band structure [Fig. 2(a,c)]. The spin Berry curvature, in contrast, does not keep the same profile upon rotation of magnetization [Fig. 2(b,d)]. Similarly for fcc-Ni $\Omega^0_{zx}$ rotates along with the band structure [Fig. 2(c,g)] when the magnetization direction is changed from $z$ to $x$ whereas $\Omega^3_{yx}$ changes its profile [Fig. 2(f,h)]. The region of non-zero $\Omega^3_{yx}$ increases when the magnetization is rotated, which causes the increase of the spin Hall conductivity.

FIG. 3. (a-f) Band structure (a,b), Berry curvatures $\Omega^0_{yx}$ (c) and $\Omega^0_{zy}$ (d), and spin Berry curvature $\Omega^3_{yx}$ (e,f) plotted along selected $k$-paths, $H(100)$-$\Gamma$-$H'(001)$, with two different magnetization configurations. The magnetization points along $z$ (a,c,e) and $x$ (b,d,f)-$m_x$. The character of the spinor state is coded with color, where red (blue) represents majority (minority) spin.

Projections of $\Omega^0_{zx}$, $\Omega^0_{yx}$ and $\Omega^3_{yx}$ along selected symmetric $k$-paths (i.e. $\Gamma - H$ and $\Gamma' - H'$[32]) with the two magnetization configurations are displayed in Fig. 3 for bcc-Fe. Large contributions to the Berry and the spin Berry curvatures are found in $k$ points where two degenerate or nearly degenerate states cross the Fermi level. In the parallel configuration (magnetization along $z$) the states consisting the band can be characterized by either the majority states (red lines in Fig. 3(a)) or the minor-
ity states (blue lines). If the relevant Bloch states have their spin direction aligned with the magnetization, the off-diagonal components of the charge velocity operator matrix \( \langle \hat{v}_i^0 | \mathbf{n}, \mathbf{n}' \rangle = \langle \mathbf{k}, \mathbf{n} | \hat{v}_i^0 | \mathbf{k}, \mathbf{n}' \rangle \) and the spin velocity operator matrix \( \langle \hat{v}_j^3 | \mathbf{n}, \mathbf{n}' \rangle \) vanish and they both reduce to a diagonal matrix. Under such circumstance, the matrix elements of the charge velocity and the spin velocity operators are nearly identical up to a sign change. For example, if the spinor states of the two degenerate bands both point along +z, i.e. \( \chi_{q,n} = \chi'_{q,n'} = (1, 0) \), the upper left component of \( \langle \hat{v}_i^0 | \mathbf{n}, \mathbf{n}' \rangle \) and \( \langle \hat{v}_j^3 | \mathbf{n}, \mathbf{n}' \rangle \) are identical, while the other three components are zero. The peaks/valleys of \( \Omega_{yx}^0 \) and \( \Omega_{yx}^3 \) thus coincide at the same \( k \) point in the parallel configuration, as evident from the plots shown in Figs. 3(c,e).

In the orthogonal configuration (magnetization pointing along \( x \)), the spin character of the states in most of the Brillouin zone is mixed with majority and minority states since the spin quantization axis is fixed along \( z \). This is displayed by the light blue/light red colors of the states shown in Fig. 3(b). Note that the spin quantization axis defines the spin direction of the conduction electrons that we look for the spin Hall effect. The corresponding Berry and spin Berry curvatures are plotted in Figs. 3(d,f). In contrast to the parallel configuration, the \( k \) points where the peaks/valleys occur for the \( \Omega_{yx}^0 \) and \( \Omega_{yx}^3 \) are different in the orthogonal configuration.

As evident above, the spin Berry curvature \( \Omega_{yx}^3 \) exhibits different profile when the magnetization direction rotated from the parallel to the orthogonal configuration. Here we show that the large change of \( \Omega_{yx}^3 \) is caused by the rotation of spinor state polarization. Let us assume a general spinor for the Bloch state when the magnetization points along +z, i.e. \( | \mathbf{k}, \mathbf{n} \rangle_z = C_n(\mathbf{k}) \left( \cos \frac{\beta}{2} \sin \frac{\alpha}{2} \right) \).

Upon rotation of the magnetization from +z to +x, the Bloch state becomes: \( | \mathbf{k}, \mathbf{n} \rangle_x = C_n(\mathbf{k}) \left( \cos \frac{\beta}{2} + \sin \frac{\alpha}{2} \right) \).

The matrix elements of \( \hat{v}_i^0 \) and \( \hat{v}_j^3 \) can be calculated as

\[
\langle \mathbf{k}, \mathbf{n}_x | \hat{v}_i^0 | \mathbf{k}, \mathbf{n}_x' \rangle = \langle \mathbf{k}, \mathbf{n}_x | \hat{v}_i^0 | \mathbf{k}, \mathbf{n}_x' \rangle \cos \frac{\beta - \alpha}{2}
\]

\[
\langle \mathbf{k}, \mathbf{n}_x | \hat{v}_i^3 | \mathbf{k}, \mathbf{n}_x' \rangle = \langle \mathbf{k}, \mathbf{n}_x | \hat{v}_i^3 | \mathbf{k}, \mathbf{n}_x' \rangle \cos \frac{\beta + \alpha}{2}
\]

\[
\langle \mathbf{k}, \mathbf{n}_x | \hat{v}_i^0 | \mathbf{k}, \mathbf{n}_x' \rangle = \langle \mathbf{k}, \mathbf{n}_x | \hat{v}_i^0 | \mathbf{k}, \mathbf{n}_x' \rangle \sin \frac{\beta + \alpha}{2}
\]

where \( \alpha \) and \( \beta \) are the polar angle of the electron spin with respect to the magnetization direction for the two Bloch states, \( n \) and \( n' \), respectively. \( v_i(\mathbf{k}) \) represents the expectation value of the velocity operator with the spatial part of the Bloch state. This simple analyses show that the \( U(1) \) velocity \( \hat{v}_i^0 \) is invariant upon rotating the spinor states. Indeed, if the two spinor states are quantized along \( z \), i.e. \( \alpha = \beta = 0 \) or \( \pi \), \( \hat{v}_i^0 \) and \( \hat{v}_j^3 \) are identical up to a sign change. However, the \( SU(2) \) velocity \( \hat{v}_i^3 \) changes its magnitude from \( \cos \frac{\beta + \alpha}{2} \) to \( \sin \frac{\beta + \alpha}{2} \): the magnitude of \( \hat{v}_i^3 \) depends on the polarization of the two spinor states.

With regard to the Kubo formula (Eq. 5), the Berry curvature is the product of the matrix elements of two \( U(1) \) velocity operators. As the \( U(1) \) velocity \( \hat{v}_i^0 \) is invariant under rotation of the spinor part of the Bloch states, the Berry curvature is invariant upon rotating the magnetization. Note that the non-vanishing components of the Berry curvature, e.g. \( \Omega_{yx}^0 \) for magnetization pointing along \( z \) and \( \Omega_{yx}^0 \) for \( x \), is determined by the direction in which the \( SU(2) \) rotation symmetry is broken. In contrast, the spin Berry curvature is the product of matrix elements between the \( U(1) \) and \( SU(2) \) velocity operators. Consequently, \( \Omega_{yx}^3 \) changes its magnitude when rotating the magnetization direction that leads to changes in the spinor part of the Bloch states. Thus the spin Hall conductivity of ferromagnets become magnetization direction dependent.

It is convenient to discuss AHE and SHE in the same framework of a \( U(1) \times SU(2) \) theory, as suggested previously [24, 33]. When considering AHE in ferromagnets, the system has almost always been treated with the magnetization direction aligned along the spin quantization axis. Therefore, the \( U(1) \times SU(2) \) theory reduces to a parallel \( U(1) \) transport model [35]. For 3d transition metals with the parallel configuration, a strong correlation between the Berry curvature and the spin Berry curvature is found, for which we may consider the \( U(1) \times U(1) \) theory is a good approximation. This is also possible because the 3d transition metals with large exchange splitting do not possess large SOC that will mix the spinor states. However, when the magnetization is rotated away from the spin quantization axis, i.e. in the orthogonal configuration, the \( U(1) \times U(1) \) approximation is no longer valid.

When the system contains elements with large SOC, significant contribution to the AHC emerges from spin flipping transitions. For example, it has been reported that the AHC of 3d-Pt alloys is significantly influenced by such transitions [36]. For such systems, the \( U(1) \times U(1) \) theory is not valid. Even without the strong SOC, \( U(1) \times U(1) \) approximation is no longer valid for 3d ferromagnets when magnetization deviates from the spin quantization axis. Under such circumstance, the off-diagonal components of the spin velocity operator matrix are non-negligible: here the spin flipping transitions might also be responsible for the the magnetization direction dependent spin Hall effect.

In conclusion, we have used bcc-Fe and fcc-Ni as prototypes to study AHC and SHC in ferromagnets. Whereas the magnitude of the non-vanishing component of the AHC in ferromagnets is independent on the magnetization direction, the non-vanishing component of the SHC is highly dependent on the relative angle between the
magnetization and the conduction electron spin orientation. With the conduction electron spin orientation fixed along $z$, the SHC of bcc-Fe (fcc-Ni) increases by a factor of 4 (1.5) when the magnetization direction is rotated from $z$ to $x$. Such magnetization direction dependent SHC originates from the anisotropy of the spin current operator in the spinor space: as the spinor part of the Bloch states changes upon rotating the magnetization direction away from the conduction electron spin orientation, the matrix elements of the spin current operator with the Bloch states vary (the magnitude of matrix elements of the velocity operator remains constant upon rotation). These results show the SHC in ferromagnets have an extra handle, i.e. the magnetization direction, to control its magnitude. Further investigation is required to clarify the effect for the extrinsic contributions to the SHC.

Notes added. During preparation of this manuscript, we came across the paper published by Amin et al. which discusses similar topic.

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