Large anomalous Nernst and spin Nernst effects in noncollinear antiferromagnets 
\( Mn_3X \) (\( X = Sn, Ge, Ga \))

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(Dated: December 12, 2017)

Noncollinear antiferromagnets have recently been attracting considerable interest partly due to recent surprising discoveries of the anomalous Hall effect (AHE) in them and partly because they have promising applications in antiferromagnetic spintronics. Here we study the anomalous Nernst effect (ANE), a phenomenon having the same origin as the AHE, and also the spin Nernst effect (SNE) as well as AHE and the spin Hall effect (SHE) in noncollinear antiferromagnetic \( Mn_3X \) (\( X = Sn, Ge, Ga \)) within the Berry phase formalism based on ab initio relativistic band structure calculations. For comparison, we also calculate the anomalous Nernst conductivity (ANC) and anomalous Hall conductivity (AHC) of ferromagnetic iron as well as the spin Nernst conductivity (SNC) of platinum metal. Remarkably, the calculated ANC at room temperature (300 K) for all three alloys is huge, being 10~40 times larger than that of iron. Moreover, the calculated SNC for \( Mn_3Sn \) and \( Mn_3Ga \) is also larger, being about five times larger than that of platinum. This suggests that these antiferromagnets would be useful materials for thermoelectronic devices and spin caloritronic devices. The calculated ANC of \( Mn_3Sn \) and iron are in reasonably good agreement with the very recent experiments. The calculated SNC of platinum also agrees with the very recent experiments in both sign and magnitude. The calculated thermoelectric and thermomagnetic properties are analyzed in terms of the band structures as well as the energy-dependent AHC, ANC, SNC and spin Hall conductivity via the Mott relations.

PACS numbers:

I. INTRODUCTION

In recent two decades, spin transport electronics (spintronics) has attracted enormous interest because of its promising applications in information storage and processing and other electronic technologies. Spin current generation, detection and manipulation are three key issues in the spintronics. In this context, spin-related transport phenomena in solids especially in those materials that can provide highly spin-polarized charge current and large pure spin current, have been intensively investigated recently. The anomalous Hall effect (AHE), discovered in 1881 by Hall, and the spin Hall effect (SHE), predicted in 1971 by Dyakonov and Perel, are two principal spin-related transports and thus have received renewed interests. Intuitively, spin-up and spin-down electrons moving through the relativistic band structure of a solid experience opposite transverse velocities caused by an applied electric field. In a ferromagnet where an unbalance of spin-up and spin-down electrons exists, these opposite currents result in a spin-polarized transverse charge current and hence the (intrinsic) AHE. Therefore, the AHE is usually assumed to be proportional to the magnetization of the magnetic material. In a nonmagnetic material where spin-up and spin-down electrons are equal in numbers, this process gives rise to a pure transverse spin current, and this is known as the (intrinsic) SHE. The SHE is particularly important for spintronics because it enables us to generate, detect and control spin current without magnetic field or magnetic materials. Furthermore, the pure spin current is dissipationless and is thus especially useful for the development of low power-consumption nanoscale spintronic devices.

Interestingly, Chen et al. recently showed that large AHE could occur in noncollinear antiferromagnets without net magnetization such as cubic \( Mn_3Ir \). This surprising result arises from the fact that in a three-sublattice kagome lattice with a noncollinear triangle antiferromagnetic structure, not only the time-reversal symmetry \( (T) \) is broken but also there is no spatial symmetry operation \( (S) \) which, in conjunction with \( T \), is a good symmetry that preserves the Kramers theorem. Subsequently, large AHE was observed in hexagonal noncollinear antiferromagnets \( Mn_3Sn \) and \( Mn_3Ge \). In the meantime, large SHE was predicted in noncollinear antiferromagnets \( Mn_3X \) (\( X = Sn, Ge, Ir \)) and was also observed in \( Mn_3Ir \). All these fascinating findings suggest that these noncollinear antiferromagnets may find exciting applications in spintronics, an emergent field called antiferromagnetic spintronics. Antiferromagnetic spintronics has been attracting increasing attention in recent years because antiferromagnetic materials have several advantages over ferromagnetic materials. In particular, antiferromagnetic elements would not magnetically affect their neighbors and are insensitive to stray magnetic fields. Moreover, antiferromagnets have faster spin dynamics than ferromagnets, and this would lead to ultra-
In a ferromagnet, the charge Hall current could also arise when a temperature gradient ($\nabla T$) instead of an electric field, is applied. This phenomenon, due to the simultaneous presence of the spin-orbit coupling (SOC) and net magnetization in the ferromagnet, is referred to as the anomalous Nernst effect (ANE)\textsuperscript{17–19}. Similarly, a temperature gradient could also generate the spin Hall current in a nonmagnetic material, and this is known as the spin Nernst effect (SNE)\textsuperscript{20}. Clearly, materials that exhibit large ANE and SNE would have useful applications for spin thermo-electronic devices driven by heat, a new field known as spin caloritronics\textsuperscript{21}. This offers exciting prospects of ‘green’ spintronics powered by, e.g., waste ohmic heat. Since the ANE and SNE, respectively, have the same physical origins as the AHE and SHE, one could expect significant ANE and SNE in the above-mentioned noncollinear antiferromagnets as well. In other words, noncollinear antiferromagnets \textit{Mn}_3\textit{X} (\textit{X} = Sn, Ge, Ga) could also be useful materials for developing antiferromagnetic spin caloritronics. Nevertheless, no investigation of the SNE in noncollinear antiferromagnets has been reported and only two reports on the measurement of the ANE in \textit{Mn}_3Sn appeared very recently\textsuperscript{22,23}. 

In this paper, therefore, we perform an \textit{ab initio} study on the ANE and SNE in hexagonal noncollinear antiferromagnets \textit{Mn}_3Ga, \textit{Mn}_3Ge and \textit{Mn}_3Sn (Fig. 1), based on the density functional theory (DFT) with the generalized gradient approximation (GGA)\textsuperscript{22,24}. For comparison, we also study the ANE in bcc Fe, a ferromagnetic transition metal having large AHE\textsuperscript{25}, and the SNE in fcc Pt, a heavy nonmagnetic transition metal exhibiting gigantic SHE\textsuperscript{22}. Indeed, we find that the anomalous Nernst conductivity at room temperature of all three alloys is large, being more than ten times larger than that of bcc Fe. The spin Nernst conductivity of \textit{Mn}_3Ga and \textit{Mn}_3Sn is larger than that of fcc Pt. The rest of this paper is organized as follows. In the next section, we briefly describe the Berry phase formalism for calculating the intrinsic Hall and Nernst conductivities as well as the computational details. Section III consists of three subsections. We first present the calculated total energy and magnetic properties of two low-energy noncollinear antiferromagnetic structures [Figs. 1(c) and 1(d)] of \textit{Mn}_3\textit{X} and also compared our results with available previous experimental and theoretical reports in Subsec. III A. We then report the calculated anomalous Nernst conductivity as well as anomalous Hall conductivity for these magnetic structures in Subsec. III B. We finally present the calculated spin Nernst conductivity and also spin Hall conductivity in Subsec. III C. Finally, the conclusions drawn from this work are summarized in Sec. IV.

![FIG. 1: (Color online) (a) Layered hexagonal (\textit{D}_3h\textsubscript{h}) structure of \textit{Mn}_3\textit{X} (\textit{X} = Sn, Ge, Ga) with (b) the associated hexagonal Brillouin zone (BZ). (c) Type A and (d) type B antiferromagnetic configurations considered in this paper. Both magnetic structures have an orthorhombic symmetry and thus their irreducible BZ wedge (IBZW) \textit{i.e.}, the trapezoid prism indicated by the blue dashed lines in (b) \textit{is} three times larger than the hexagonal IBZW \textit{i.e.}, the triangle prism indicated by the blue dashed lines in (b)]. The vertical [horizontal] black dashed line in (c) [(d)] denotes the mirror plane.](image)

II. THEORY AND COMPUTATIONAL METHOD

Here we consider ordered \textit{Mn}_3Ga, \textit{Mn}_3Ge and \textit{Mn}_3Sn alloys in the layered hexagonal \textit{DO}_{19} (\textit{P6}_3\textit{mmc} or \textit{D}_3h\textsubscript{h}) structure [see Fig. 1(a)] and use the experimental lattice constants of \textit{a} = 5.36 Å and \textit{c} = 4.33 Å, \textit{a} = 5.34 Å and \textit{c} = 4.31 Å, and \textit{a} = 5.66 Å and \textit{c} = 4.53 Å, respectively. The primitive unit cell contains two layers of \textit{Mn} triangles stacked along the \textit{c}-axis, and in each layer the three \textit{Mn} atoms form a kagome lattice with the \textit{X} atom located at the center of each hexagon (Fig. 1). The total energy and electronic structure are calculated based on the DFT with the GGA in the form of Perdew-Burke-Ernzerhof\textsuperscript{24}. The accurate projector-augmented wave (PAW) method\textsuperscript{25}, as implemented in the Vienna \textit{ab initio} simulation package (\textit{vasp})\textsuperscript{29,30}, is used. The fully relativistic PAW potentials are adopted in order to include the SOC. The valence configurations of \textit{Mn}, \textit{Sn}, \textit{Ge} and \textit{Ga} atoms taken into account in the calculations are 3\textit{d}^5\textit{S}^1, 4\textit{d}^{10}5\textit{s}^25\textit{p}^2, 3\textit{d}^{10}4\textit{s}^24\textit{p}^2 and 3\textit{d}^{10}4\textit{s}^24\textit{p}^1, respectively. A large plane-wave cutoff energy of 350 eV is used throughout. In the self-consistent electronic structure calculations, a fine \Gamma-centered \textit{k}-point mesh of 20\times20\times20 \textit{i.e., 2112 \textit{k}-points over the orthorhombic irreducible Brillouin zone wedge (IBZW) (see Fig. 1)] is adopted for the Brillouin zone (BZ) integration using the tetrahedron method\textsuperscript{31}. The anomalous Hall conductivity (AHC) and anomalous Nernst conductivity (ANC) are calculated based on
the elegant Berry-phase formalism. Within this Berry-phase formalism, the AHC \( \sigma^A_{ij} = J^i_e/E_j \) is simply given as a BZ integration of the Berry curvature for all the occupied bands,

\[
\sigma^A_{ij} = -\frac{e^2}{h} \sum_n \int_{BZ} \frac{dk}{(2\pi)^3} f_{kn} \Omega^A_{ij}(k),
\]

\[
\Omega^A_{ij}(k) = -\sum_{n',n \neq n} 2\text{Im} \left\{ \langle kn'|v_i|kn \rangle \langle kn'|v_j|kn \rangle \right\} (\epsilon_{kn} - \epsilon_{kn'})^2,
\]

where \( f_{kn} \) and \( \Omega^A_{ij}(k) \) are the Fermi distribution function and the Berry curvature for the \( n \)th band at \( k \), respectively. \( i \) and \( j \) \( (x,y,z) \), and \( i \neq j \). \( J^i_e \) is the \( i \)-component of the charge current density \( \mathbf{J} \) and \( E_j \) is the \( j \)-component of the electric field \( \mathbf{E} \). Moreover, the ANC \( (\alpha^A_{ij} = -J^i_e/\nabla \times T) \) can be written as

\[
\alpha^A_{ij} = \frac{1}{T} e \sum_n \int_{BZ} \frac{dk}{(2\pi)^3} \Omega^A_{ij}(k) \times \left[ (\epsilon_{kn} - \mu)f_{kn} + k_B T \ln(1 + e^{-\beta(\epsilon_{kn} - \mu)}) \right],
\]

where \( \mu \) is the chemical potential and \( k_B \) is the Boltzmann constant.\(^{19,33}\)

The Berry curvature \( \Omega^A_{ij}(k) \) can be considered as a pseudovector, just like the spin, and thus can be written as \( [\Omega^A_{ij}(k), \Omega^B_{ij}(k), \Omega^C_{ij}(k)] = [\Omega^A_{ij}(k), \Omega^B_{ij}(k), \Omega^C_{ij}(k)] \). Thus, \( \Omega_n(k) = \Omega_n(-k) \) if the system has spatial inversion symmetry \( (P) \) and \( \Omega_n(k) = -\Omega_n(-k) \) if it has \( T \) symmetry.\(^{26}\) Obviously, if the system has both \( P \) and \( T \) symmetries, \( \Omega_n(k) \) becomes identically zero. The AHC and ANC are also pseudovectors and can be written as \( [\sigma^A_{ij}, \sigma^A_{ij}, \sigma^A_{ij}] = [\sigma^A_{ij}, \sigma^A_{ij}, \sigma^A_{ij}] \) and \( [\alpha^A_{ij}, \alpha^A_{ij}, \alpha^A_{ij}] = [\alpha^A_{ij}, \alpha^A_{ij}, \alpha^A_{ij}] \), respectively.

Similarly, the spin Hall conductivity \( (\sigma^S_{ij} = J^i_s/E_j) \) is given by a BZ integration of the spin Berry curvature \( \Omega^S_{ij}(k) \) for all the occupied bands,

\[
\sigma^S_{ij} = -e \sum_n \int_{BZ} \frac{dk}{(2\pi)^3} f_{kn} \Omega^S_{ij}(k),
\]

\[
\Omega^S_{ij}(k) = -\sum_{n',n \neq n} 2\text{Im} \left\{ \langle kn'|\{\tau_s,v_i\}|kn \rangle \langle kn'|v_j|kn \rangle \right\} (\epsilon_{kn} - \epsilon_{kn'})^2,
\]

where \( s \) denotes the spin direction and \( \tau_s \) is a Pauli matrix.\(^{26}\) Then the spin Nernst conductivity \( (\alpha^S_{ij} = -J^i_s/\nabla s T) \) can be written as

\[
\alpha^S_{ij} = \frac{1}{T} e \sum_n \int_{BZ} \frac{dk}{(2\pi)^3} \Omega^S_{ij}(kn) \times \left[ (\epsilon_{kn} - \mu)f_{kn} + k_B T \ln(1 + e^{-\beta(\epsilon_{kn} - \mu)}) \right],
\]

where \( J^i_s \) denotes the \( i \)-component of the spin current density \( \mathbf{J} \) with spin being along the \( s \)-axis.

In the AHC, SHC, ANC and SNC calculations, the velocity \( \{\langle kn|v_i|kn'\rangle\} \) and spin-velocity \( \{\langle kn|\{\tau_s,v_i\}|kn'\rangle\} \) matrix elements are obtained from the self-consistent electronic structure within the PAW formalism. To obtain accurate AHC, SHC, ANC and SNC, a dense \( k \)-point mesh would be needed.\(^{25,35}\) Therefore, we use a very fine mesh of 97344 \( k \)-points on the magnetic IBZ (1/8 BZ), together with the tetrahedron method.\(^{23}\) This is equivalent to a large number of \( k \)-points of \( \sim 778752 \) in the full BZ, and corresponds to the division of the \( \Gamma \) line into \( n_d = 50 \) intervals. Further calculations using \( n_d = 20, 30 \) and 40 (i.e., 7260, 22272, 51597 \( k \)-points in the IBZ, respectively) indicate that the AHC, SHC, ANC and SNC obtained using \( n_d = 50 \) converge to within a few \%. Indeed, the curves of AHC, SHC, ANC and SNC as a function of energy (see Figs. 3-5 below) and also the curves of ANC and SNC as a function of temperature (see Fig. 6 below) obtained with \( n_d = 40 \) and 50 are indistinguishable. Moreover, the calculated AHC, SHC, ANC and SNC versus the inverse of the number \( (N_k) \) of \( k \)-points in the IBZ are plotted and fitted to a straight line to get the converged theoretical values listed in Table II below (i.e., the extrapolated values at \( N_k = \infty \)) (see Refs.\(^{22,37}\)). Note that the differences between the converged theoretical AHC, SHC, ANC and SNC values and the corresponding \( n_d = 50 \) values are within a few \%. As mentioned before, we also calculate the AHC and ANC of ferromagnetic bcc Fe and the SNC of nonmagnetic fcc Pt for comparison. In the calculation of the AHC and ANC of bcc Fe, we also adopt a very fine mesh of 360396 \( k \)-points on the magnetic IBZ (1/16 BZ). In the SHC and SNC calculations for fcc Pt, a very fine grid of 253044 \( k \)-points on the magnetic IBZ (1/16 BZ) is used.

### III. RESULTS AND DISCUSSION

The energetics of many possible magnetic configurations for MnSn in the hexagonal DO\(_{19}\) structure has already been investigated with the \textit{ab initio} density functional calculations.\(^{25,40}\) Therefore, in this paper we consider only two low-energy noncollinear triangular antiferromagnetic configurations for MnSn (\( X = \text{Sn, Ge, Ga} \)) \( (\text{see Fig. 1(c) and Fig. 1(d) in Ref.}\(^{39})\), namely, type A and type B configurations as illustrated in Fig. 1(c) and Fig. 1(d), respectively. For comparison, the antiferromagnetic state (FM) of MnSn with magnetic moments in the \( \hat{x} \)-direction is also investigated.

#### A. Magnetic properties

The calculated total energies and spin magnetic moments are listed in Table II together with the reported experimental values. Table II shows that in all three alloys, magnetic structure A has a lower energy than magnetic structure B, although the total energy difference is in the order of ~0.01 meV. This agrees with the magnetic structure observed in earlier neutron diffraction experiments on MnSn, MnSnGe and MnSnGa. In
TABLE I: Calculated total energy \( (E_t) \) and total spin magnetic moment \( (m_t^s) \) as well as averaged Mn spin magnetic moment \( (m_{\text{Mn}}^s) \) for the A and B magnetic structures of Mn\(_3\)X \((X = \text{Sn, Ge, Ga})\). Total magnetic moments are parallel to the \( \hat{x} \)-axis in configuration A but to the \( \hat{y} \)-axis in configuration B. The X atoms have a nearly zero magnetic moment (being less than 0.01 \( \mu_B \)) and thus are not listed. Note that there are two formula units [i.e., 2(Mn\(_3\)X)] per unit cell. For comparison, the results of the magnetic moment direction-constrained calculation for Mn\(_3\)Ga in configuration A (denoted A*) and the ferromagnetic calculation for Mn\(_3\)Ga with the magnetic moments in the \( \hat{x} \)-direction (denoted FM) are given as well. Some previously reported total and Mn spin moments are also listed for comparison.

|          | \( E_t \) (meV/cell) | \( m_{\text{Mn}}^s \) (\( \mu_B/\text{atom} \)) | \( m_t^s \) (\( 10^{-3} \mu_B/\text{cell} \)) |
|----------|-------------------|-----------------|-----------------|
| Mn\(_3\)Sn | A 0.0 3.13, 3.0\(^a\) | 0.1, 12\(^b\) | |
|          | B 0.03 3.13 | 22 | |
| Mn\(_3\)Ge | A 0.0 2.70, 2.4\(^a\) | 0.9, 42\(^d\) | |
|          | B 0.03 2.68 | 2.3, 30\(^d\) | |
| Mn\(_3\)Ga | A* 0.00 2.75, 2.4\(^f\) | 11.3 | |
|          | A 0.01 2.73 | 10.9 | |
|          | B 0.01 2.73 | 10.9 | |
|          | FM 855 2.18 | 13019 | |

\(^a\)Ref. 41 (experiment), \(^b\)Ref. 11 (experiment), \(^c\)Ref. 42 (experiment), \(^d\)Ref. 13 (experiment), \(^e\)Ref. 12 (experiment).

Table II lists the calculated anomalous Nernst conductivity (\( \sigma_{ij}^A \)), anomalous Hall conductivity (\( \sigma_{ij}^H \)) and density of states at the Fermi level [\( N(E_F) \)] of Mn\(_3\)X \((X = \text{Sn, Ge, Ga})\) alloys. As discussed before, the AHC and ANC are pseudovectors, just like the total magnetic moment. Thus, in the A (B) magnetic structure, only \( m_{t,y} \) (\( \sigma_{yx}^A \)) and \( m_{t,z} \) (\( \sigma_{zx}^A \)) can be nonzero. This can also be seen from the k-space distribution of the Berry curvature \( \Omega(k) = \Omega^{x}(k), \Omega^{y}(k), \Omega^{z}(k) \), as displayed in Fig. 2 for configuration A of Mn\(_3\)Sn. Figure 2(a) shows that in the \( k_xk_y \) (i.e., \( k_z = 0 \)) plane, \( \Omega^{x}(k) \) is an odd function of \( k_x \) while \( \Omega^{z}(k) \) is an even function of \( k_x \). In Fig. 2(b), \( \Omega^{y}(k) \) is found to be an odd function of \( k_x \) while \( \Omega^{z}(k) \) is again an even function of \( k_x \) in the \( k_xk_z \) (i.e., \( k_y = 0 \)) plane. Consequently, Eqs. (1) and (2) would indicate that \( \sigma_{yx}^A \) and \( \sigma_{zx}^A \) as well as \( \sigma_{xx}^A \) and \( \sigma_{xy}^A \) should be zero. The present results (Table II) are consistent with these symmetry properties. It is also clear from Table II that the AHC, ANC and \( N(E_F) \) for both A and B configurations are very similar. This is consistent with the fact that the two configurations have nearly degenerate total energies and very similar magnetic properties (Table I).

The calculated \( \sigma_{xx}^A \) and \( \sigma_{xy}^A \) of iron metal are also listed there for comparison. Table II shows that the AHC of all the Mn\(_3\)X alloys is rather large, being in the same order of magnitude as that of ferromagnetic iron with a large net magnetic moment of 2.27 \( \mu_B/\text{atom} \). Remarkably, all the Mn\(_3\)X alloys have a huge ANC, which is 10\(\sim\)40 times larger than that of Fe (Table II). This strongly suggests that these noncollinear antiferromag-
TABLE II: Calculated density of states at the Fermi level \(N(E_F)\) (states/eV/spin/f.u.), anomalous Hall conductivity (AHC; \(\sigma_{xy}^A\)) \((\sigma_{yz}^A, \sigma_{zx}^A)\) and anomalous Nernst conductivity (ANC; \(\sigma_N^A\)) \((\alpha_{yz}^A, \alpha_{zx}^A)\) as well as spin Hall conductivity (SHC) \((\sigma_{xy}^S)\) and spin Nernst conductivity (SNC) \((\alpha_{yz}^S, \alpha_{zx}^S)\) of Mn₃X \((X = \text{Sn, Ge, Ga})\). For comparison, the calculated related properties of bcc Fe \((\sigma_{xy}^F, \alpha_{yz}^F)\) and fcc Pt \((\sigma_{xy}^F, \alpha_{yz}^F)\) are also listed. Note that ANC and SNC listed here were calculated at temperature \(T = 300\) K. The ANC for Mn₃Sn in brackets were calculated at \(T = 210\) K and the SNC for fcc Pt in brackets were calculated at \(T = 255\) K. For comparison, the results of the magnetic moment direction-constrained calculation for Mn₃Ga in configuration A (denoted A⁺) and the ferromagnetic calculation for Mn₃Ga with the magnetic moments in the \(\hat{x}\)-direction (denoted FM) are given as well. Some previous experimental results are also listed for comparison.

| \(N(E_F)\) \((\text{S/cm)}\) | \(\sigma_{xy}^A\) \((\text{S/cm}\mu\text{eV})\) | \(\sigma_{xy}^S\) \((\text{A/m$\mu$K})\) | \(\sigma_{yz}^A\) \((\text{h/eV}/\text{cm$^2$})\) | \(\sigma_{yz}^S\) \((\text{h/eV}/\text{cm$^2$})\) | \(\alpha_{yz}^A\) \((\text{h/eV}/\text{A/m$\mu$K})\) | \(\alpha_{yz}^S\) \((\text{h/eV}/\text{A/m$\mu$K})\) |
|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| Mn₃Sn | A | 1.96 | -132, -68a,-90b | 656 | -46.8 (-1.16), -39c \(-, 0.28c\) | 72 | -845 | 7.7 |
| B | 1.96 | -132, -126b,-80b | 644 | -4.7 (-1.18), -32b | 74 | -834 | 7.5 |
| Mn₃Ge | A | 2.37 | -298, 310d,150e | -9020 | -6.4 | 56 | 691 | 1.02 |
| B | 2.38 | -298, 380d,500e | -8289 | -6.4 | 63 | 1000 | 0.63 |
| Mn₃Ga | A | 5.99 | -104 | -3722 | 17.1 | -219 | -5323 | 7.3 |
| A⁺ | 5.99 | -106 | -3697 | 17.3 | -219 | -5134 | 7.4 |
| B | 5.99 | -103 | -3953 | 17.0 | -241 | -3561 | 6.6 |
| FM | 6.82 | 181 | -12836 | -14.0 | -678 | -10601 | 3.2 |
| bcc Fe | 1.11 | 708,1200f | -230 | 0.40,1.8g | - | - | - |
| fcc Pt | 1.75 | - | - | - | 2139 | 1214 | -1.11 \(-0.92),-1.57f |

\(a\)Ref. 11 (experiment at 50 K), \(b\)Ref. 22 (experiment at 210 K), \(c\)Ref. 23 (experiment at 200 K), \(d\)Ref. 12 (experiment at 10 K), \(e\)Ref. 13 (experiment at 2 K), \(f\)Ref. 22 (experiment at 300 K). \(^{g}\)Extracted from the experiment at 255 K \(\text{(Ref. 16).}\)

nets would find promising applications in thermoelectric devices, heat nanosensors and also spin caloritronics.

One may wonder whether the nonzero ANC and AHC are caused by the presence of the small net magnetization in these noncollinear antiferromagnetic structures, as in the case of ferromagnets where the ANC and AHC are proportional to the net magnetization. To address this issue, we perform the magnetic moment direction-constrained GGA calculation for the A structure of Mn₃Ga in order to make the total magnetic moment vanished. The results of this calculation are listed in Tables I and II. Table II shows that the resultant ANC and AHC remain nearly unchanged, although the net magnetic moment is reduced by a factor of \(~20\) (Table I). Moreover, we also carry out the GGA calculation for Mn₃Ga in the ferromagnetic state (FM) with magnetization along the \(\hat{z}\)-axis. Interestingly, although the total magnetic moment of the FM state is three orders of magnitude larger than that of the A structure (Table I), the ANC gets reduced by 20 %, compared with that of the A structure.

The calculated ANC \((\alpha_{yz}^A)\) and AHC \((\sigma_{yz}^A)\) of magnetic structure A as a function of the Fermi energy \((E_F)\) as well as the relativistic band structure are plotted in Fig. 3 for Mn₃Sn, in Fig. 4 for Mn₃Ge and in Fig. 5 for Mn₃Ga. Figure 3 shows that for up to 0.33 eV above the \(E_F\), the \(\sigma_{yz}^A\) of Mn₃Sn is negative and rather flat with small ripples. However, if the Fermi energy is lowered to \(-0.114\) eV, one sees a very pronounced negative peak in \(\sigma_{yz}^A\). The peak \(\sigma_{yz}^A\) value is \(-979\) S/cm. To reach this energy level, the number of valence electrons should be reduced by 0.206 per formula unit (f.u.), indicating substitution of \(~20\) % of Sn by In or Ga. Examination of the calculated band-resolved Berry curvatures suggests that this peak arises predominantly from the large \(\Omega_{yz}\) on the top valence band in the vicinity of the gap at M-point [see Fig. 3(a)]. The shape of the \(\sigma_{yz}^A\) versus \(E_F\) curve in Mn₃Ge [Fig. 4(b)] is similar to that of Mn₃Sn [Fig. 3(b)], and this is understandable because both alloys are isoelectronic. Mn₃Ga has roughly the same \(\sigma_{yz}^A\) versus \(E_F\) curve [Fig. 5(b)] as that of Mn₃Ge and Mn₃Sn except that the Fermi level is now about 0.25 eV lower mainly because Mn₃Ga has one less valence electron.

To understand the features in the \(\alpha_{yz}^A\) versus \(E_F\) curve, one should note that at low temperatures, Eq. (2) can be simplified as the Mott relation,

\[\alpha_{yz}^A = -\frac{2}{3} \frac{k_B^2 T}{e} \sigma_{yz}^A \mu' \]  

which relates the ANC to the energy derivative of the ANC. This Mott relation roughly explains why in Mn₃Sn [Fig. 3(c)] there is a prominent peak in \(\alpha_{yz}^A\) at \(-0.070\) eV, where \(\sigma_{yz}^A\) has a steep slope [Fig. 3(b)]. The peak \(\alpha_{yz}^A\) value is as large as \(-19\) A/m,K at 300 K. One could reach this point by reducing the valence electrons by 0.13 electron per Mn₃Sn, i.e., by merely substituting 13 % Sn with In or Ga. As mentioned before, \(\sigma_{yz}^A\) is rather flat above the Fermi level [Fig. 3(b)], and this explains why \(\alpha_{yz}^A\) becomes nearly zero slightly above the \(E_F\) [Fig. 3(c)]. We have also calculated the ANC of all the alloys as a function of temperature \((T)\) and the results are displayed in Fig. 6(a) together with the calculated \(T\)-dependent \(\sigma_{yz}^A\) of bcc Fe. Figure 6(a) shows that at high temperature \((300\sim400\) K) Mn₃Ga has a very large \(\alpha_{yz}^A\), being up to \(~20\) A/m,K which is 50 times larger than that of bcc Fe. The \(\alpha_{yz}^A\) of Mn₃Ga decreases steadily with decreasing \(T\) and eventually approaches zero at \(~50\) K. The magnitude of the ANC of Mn₃Sn and Mn₃Ge is also large.
at high temperatures (e.g., \( \sim 10 \) A/m-K at \( T = 400 \) K) but the sign of the ANC is negative, being opposite to that of Mn$_3$Ga. The magnitudes of the ANC of Mn$_3$Sn and Mn$_3$Ge decrease monotonically as \( T \) decreases and change sign at 175 K and 200 K, respectively. As \( T \) further cools, the ANC of Mn$_3$Ge increases steadily and reaches 5.2 A/m-K at 50 K, while that of Mn$_3$Sn stays around 0.6 A/m-K with small fluctuations. Because of their large ANC at room temperature [being at least one order of magnitude larger than that of bcc Fe (see Table II)], all three Mn$_3$X alloys could serve as a thermoelectric material for spin caloritronics.

To examine the validity of the Mott relation [Eq. (5)], we calculated the energy derivative of the AHC for all the alloys and bcc Fe, as listed in Table II. The ANC at 100 K calculated using Eq. (5) and the energy derivatives of the AHC are shown in Fig. 6(a). Figure 6(a) indicates that the ANC values calculated this way agree in sign with those calculated directly using Eq. (2) for Mn$_3$Sn, Mn$_3$Ge and bcc Fe. However, the magnitudes differ significantly. At 300 K, the ANC for all Mn$_3$X alloys estimated using Eq. (5) would differ in sign from those from Eq. (2) (listed in Table II). We note that in the magnetized Pt and Pd, at 100 K the \( \alpha_{\text{N}}^{\text{A}} \) calculated using the Mott relation [Eq. (5)] and directly from Eq. (2) agree quantitatively, and even at 300 K they agree with each other quite well.

The band structures of magnetic structures A and B of all three alloys are almost identical and thus their band structures for the B configuration are not presented in this paper. Furthermore, the two magnetic configur-
actions for each alloy have similar AHC and ANC as a function of energy and hence the AHC and ANC as a function of energy of the B configuration are not displayed here either. The present band structures of Mn$_3$Sn (Fig. 3) and Mn$_3$Ge (Fig. 4) are in good agreement with the previous GGA results\textsuperscript{14,47}. The present (Fig. 5) and previous GGA band structures for Mn$_3$Ga also agree quite well along all the high symmetry lines except the KM line where the two band structures differ quite significantly.

As mentioned before, the AHE in Mn$_3$Sn and Mn$_3$Ge in noncollinear antiferromagnetic states have been experimentally investigated by several groups\textsuperscript{22,23}. The calculated AHC (132 S/cm) for Mn$_3$Sn in configuration B agrees well with the measured value (126 S/cm at 50 K) reported in Ref. [11], although the theoretical AHC (132 S/cm) in configuration A is nearly twice as large as the measured value (68 S/sm) (see Table II). The calculated AHC for Mn$_3$Ge in both configuration A and B is also in good agreement with the experimental value at 10 K reported in Ref. [12], although for configuration B it is about 30% smaller than the measured one (500 S/cm at 2 K) presented in Ref. 13 and for configuration A it is twice as large as the measured one.\textsuperscript{14} All these suggest that the anomalous Hall effect in these alloys is dominated by the intrinsic mechanism due to the nonzero Berry curvatures in the momentum space.\textsuperscript{22,23} This is also the conclusion drawn in Ref. [22] based on the experimental examination on the validity of the Wiedemann-Franz law. The AHC of Mn$_3$Sn (Mn$_3$Ge) presented in Table II is in excellent agreement with the GGA result of 133 (330) S/cm of Mn$_3$Sn (Mn$_3$Ge) reported in Refs. [14,47].

However, unlike the AHE case, so far merely two papers very recently reported on the experiments on the ANE in Mn$_3$Sn\textsuperscript{22,23} It was found that the ANE signals are significant and easily detectable.\textsuperscript{22,23} Furthermore, the thermal and Nernst conductivities was found to correlate according to the Wiedemann-Franz law, indicating the intrinsic origin of the ANE. Overall, this is consistent with our finding of large intrinsic ANE in these alloys. Also the measured and calculated ANC at \(\sim 210\) K agree in sign with respect to that of AHC, although the measured ANC (0.39 and 0.28 A/m-K) for configuration A is a few times smaller than the calculated ANC (1.16 A/m-K) (Table II). Nevertheless, experimentally, the ANC and AHC were found to decrease steadily as the \(T\) is increased from 200 K to 400 K\textsuperscript{22,23} in contrast to the monotonical increase of the calculated ANC with \(T\) (Fig. 6(a)). This significant discrepancy could arise from several reasons. First of all, the temperature range of 200~400 K is close to the antiferromagnetic transition (\(T_N\)) and consequently the magnetism gets weaker as the \(T_N\) is approached. In the theoretical calculation, however, the \(T = 0\) magnetism is assumed and the \(T\)-dependence enters only through the Fermi function [see Eq. (2)]. Secondly, although the ANC is calculated directly from the band structure [see Eq. (2)], experimentally, the ANC cannot be measured directly and thus is estimated using measurable longitudinal ((\(\rho_{ij}\)) and Hall ((\(\rho_{ij}\))) resistivities as well as Seebeck (\(S_{ij}\)) and Seebeck-Nernst (\(S_{ij}\)) coefficients via\textsuperscript{22,23}

\[
\alpha^A_{yz} = \frac{\rho_{zz} S_{yz} - \rho_{yz} S_{zz}}{\rho_{yy} \rho_{zz} - \rho_{yz} \rho_{zy}} \approx \frac{\rho_{zz} S_{yz} - \rho_{zz} S_{yz}}{\rho_{yy} \rho_{zz}}. \tag{6}
\]

Clearly, to obtain accurate estimated ANC, all these quantities must be accurately measured on the same sample, but this often is not the case. Given all these complications, we believe that the level of agreement between the experiment and calculation is quite good. Table II shows that the experimental ANC of iron at 300 K also reported in [22] is \(\sim 1.8\) A/m-K, being four times larger than the present theoretical ANC (0.4 A/m-K). Furthermore, a previous GGA calculation of the intrinsic ANC\textsuperscript{22} of iron gave a value of 0.16 A/m-K, being more than two times smaller than the present GGA result. Further experiments on the ANE and AHE on these alloys are clearly needed.

C. Spin Nernst effect

The SNC ((\(\sigma^s_{xy}\), \(s, i, j = x, y, z\)) and SHC ((\(\sigma^s_{xy}\)) are third-order tensors. A recent symmetry analysis\textsuperscript{14} showed that only elements ((\(\sigma^s_{yz}\), \(\sigma^s_{yz}\), \(\sigma^s_{y}\)) and \(\sigma^s_{y}\)) can be nonzero. Furthermore, the \(ab\) \textit{initio} calculations of the SHC of Mn$_3$X \((X = Sn, Ge, Ga)\)\textsuperscript{14} indicated that only \(\sigma^s_{yz}\) and \(\sigma^s_{y}\) are significantly nonzero. Therefore, in this paper we consider only \(\sigma^s_{yz}\) and \(\sigma^s_{y}\). The calculated \(\sigma^s_{yz}\) and \(\sigma^s_{y}\) of all Mn$_3$X alloys are listed in Table II. The \(\sigma^s_{yz}\) and \(\sigma^s_{y}\) of platinum metal\textsuperscript{33} are also listed there for comparison. Table II shows that the SHC of the Mn$_3$X alloys is rather small, compared to
that of platinum, which has the largest intrinsic SHC among transition metals.\(^7\) Remarkably, the SNC of MnSn and Mn3Ga is very large, being about five times larger than that of Pt (Table II). Mn3Ge also has a larger SNC than platinum. This shows that noncollinear antiferromagnets Mn3X (X = Sn, Ge, Ga) would be very useful materials for spin thermoelectric devices and spin caloritronics, just like Pt metal for spintronics.

The calculated SNC \(\alpha_{xy}^z\) and SHC \(\sigma_{xy}^z\) as a function of the Fermi energy \(E_F\) of Mn3Sn, Mn3Ge and Mn3Ga are displayed in Fig. 3, Fig. 4 and Fig. 5, respectively. Figures 3(b) and 4(b) show that in both Mn3Sn and Mn3Ge the \(\sigma_{xy}^z\) in the vicinity of the \(E_F\) is rather small, thus resulting in a small value at the \(E_F\) (Table II). Nevertheless, the \(\sigma_{xy}^z\) in Mn3Ge has a broad prominent peak near -0.30 eV, and the peak value is as large as -750 \(\mu\text{V/K}\) at 255 K.\(^5\) This peak can be reached by a reduction of the valence electrons of \(\sim 1.0\) e/f.u. For Mn3Ga which has one less valence electron, the \(E_F\) is lowered to just below this peak [Fig. 4(b)], thus resulting in a much larger \(\sigma_{xy}^z\) value (Table III).

To understand the features in the \(\alpha_{xy}^z\) versus \(E_F\) curve, one should note again that Eq. (4) would be reduced to

\[
\alpha_{xy}^z = -\frac{\pi^2 k_B T}{3 e} \sigma_{xy}^z (\mu)^2,
\]

which relates the SNC to the energy derivative of the SHC. This Mott relation roughly explains why in Mn3Sn [Fig. 3(c)] the \(\alpha_{xy}^z\) has a broad plateau from -0.09 eV to 0.23 eV around the \(E_F\), where \(\sigma_{xy}^z\) has more or less a constant negative slope [Fig. 3(b)]. The plateau \(\alpha_{xy}^z\) value is about 9 \((\mu\text{V/K})\) at 300 K. In Mn3Ge, the \(\alpha_{xy}^z\) is rather small in the vicinity of the \(E_F\) because \(\sigma_{xy}^z\) is rather flat (and small) (Fig. 4). Nevertheless, the \(\alpha_{xy}^z\) has a prominent negative peak at -0.21 eV [Fig. 4(c)] where \(\sigma_{xy}^z\) has a steep slope [Fig. 4(b)]. Within the rigid band model, the \(\alpha_{xy}^z\) peak could be reached by reducing the number of valence electrons by \(\sim 0.51\) e/f.u. In Mn3Ga, the \(E_F\) sits on the upper side of the pronounced peak at -0.035 eV and thus \(\alpha_{xy}^z\) is large, being as large as 14 \((\mu\text{V/K})\) at 300 K. Again, this is because the \(\sigma_{xy}^z\) has a steep slope at -0.035 eV [Fig. 5(b)].

Very recently, the SNE in platinum was studied experimentally and a large spin Nernst angle (\(\theta_{SN}\)) was observed.\(^6\) The spin Nernst angle is comparable in size but opposite in sign to the spin Hall angle (\(\theta_{SH}\)) with \(\theta_{SH}/\theta_{SN} = -0.5\) at 255 K.\(^6\) It can be shown that \(\alpha_{xy}^z = -\alpha_{xy}^z S_{xy}/(\theta_{SH}/\theta_{SN})\). Using the theoretical \(\sigma_{xy}^z = 2139\) \((\mu\text{V/K})\) (Table III) and measured Seebeck coefficient \(S_{xy}^z = -3.67\) \((\mu\text{V/K})\) at 255 K, we would obtain an estimated experimental \(\alpha_{xy}^z = -1.57\) \((\mu\text{V/K})\), agreeing quite well with the calculated value of -0.92 \((\mu\text{V/K})\) (Table III).

In Fig. 6(b), the calculated \(T\)-dependence of the SNC for all three alloys as well as Pt metal are displayed. Fig. 6(b) shows that the magnitude of the SNC of Mn3Sn is very large at high temperatures (e.g., \(\sim 10\) \((\mu\text{V/K})\)) at \(T = 400\) K. Nevertheless, the SNC decreases monotonically as the \(T\) decreases down to 50 K. Interestingly, the SNC of Pt has a very similar \(T\)-dependence, albeit with a much smaller magnitude and an opposite sign. In contrast, Mn3Ga has a smaller SNC at high temperatures (e.g., \(\sim 4.4\) \((\mu\text{V/K})\)) at \(T = 400\) K. However, the SNC of Mn3Ga increases steadily as the \(T\) is lowered, and it reaches its maximum of \(\sim 10\) \((\mu\text{V/K})\) at \(T = 175\) K. It then decreases monotonically as the \(T\) further decreases. Mn3Ge has a small SNC at high temperatures (e.g., \(\sim 1.9\) \((\mu\text{V/K})\)) at \(T = 400\) K. The SNC of Mn3Ge decreases gradually as the \(T\) decreases and changes sign at \(T = 225\) K. After passing 225 K, it further decreases as the \(T\) is lowered to 125 K, and it then increases slightly as the \(T\) decreases to 50 K.

We calculated the energy derivative of the SHC for all the alloys and fcc Pt, as listed in Table II, in order to examine the validity of the Mott relation [Eq. (7)]. The SNC at 100 K calculated using Eq. (7) and the energy derivatives of the SHC are shown in Fig. 6(b). Figure 6(b) indicates that all the SNC values calculated this way agree in sign with those calculated directly using Eq. (4). For fcc Pt, the SNC values \([-0.30\) and \(-0.31\) \((\mu\text{V/K})\)]
agree rather well. This level of agreement [-0.89 and -1.11 (ℏe)S/cm] is maintained even at 300 K. For Mn$_3$Ga (Mn$_3$Ge), the SNC value from Eq. (7) is 2.5 (five) times smaller than that from Eq. (4). For Mn$_3$Sn, the SNC values from Eq. (7) and Eq. (4) differ by one order of magnitude [Fig. 6(b)].

IV. CONCLUSIONS

We have studied theoretically the ANE, a phenomenon having the same origin as the AHE, and also the SNE as well as the AHE and SHE in noncollinear antiferromagnetic Mn$_3$X (X = Sn, Ge, Ga) based on ab initio relativistic band structure calculations. As references, we also calculate the ANC and AHC of ferromagnetic iron as well as the SNC of platinum metal. Fascinatingly, the calculated ANC at room temperature (300 K) for all three alloys is huge, being 10~40 times larger than that of iron. Further, the calculated SNC for Mn$_3$Sn and Mn$_3$Ga is also larger, being about five times larger than that of platinum. This suggests that these antiferromagnets would be useful materials for thermoelectric devices and spin caloritronic devices. The calculated ANC of Mn$_3$Sn and iron are in reasonably good agreement with the very recent experiments. The calculated SNC of platinum also agree well with the very recent experiments in both sign and magnitude. The calculated thermoelectric and thermomagnetic properties are analyzed in terms of the band structures as well as the energy-dependent AHC, ANC, SNC and SHC via the Mott relations. We hope that our interesting theoretical results would stimulate further experimental works on these noncollinear antiferromagnets.

Acknowledgments

The authors acknowledge support from the Ministry of Science and Technology and the Academia Sinica of The R.O.C. as well as the NCTS and the Kenda Foundation in Taiwan. G.Y.G thanks Qian Niu for stimulating discussions.

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1 G. A. Prinz, Science 282, 1660 (1998); S. A. Wolf, D. D. Awschalom, R. Chtchelkanova, and D. M. Treger, ibid., 294, 1488 (2001)
2 I. Zutic, J. Fabian, and S. D. Sarma, Rev. Mod. Phys. 76, 323 (2004).
3 E. H. Hall, Phil. Mag. B 12, 157 (1881).
4 M. I. Dyakonov and V. I. Perel, Sov. Phys. JETP 33, 1053 (1971).
5 N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, Rev. Mod. Phys. 82, 1539 (2010)
6 J. Sinova, S. O. Valenzuela, J. Wunderlich, C. H. Back and T. Jungwirth, Rev. Mod. Phys. 87, 1213 (2015)
7 A. Hoffman, IEEE Trans. Mag. 49, 5172 (2013).
8 S. Murakami, N. Nagaosa, and S.-C. Zhang, Science 301, 1348 (2003)
9 L. Liu, C.-F. Pai, Y. Li, H.-W. Tseng, D. C. Ralph, and R. A. Buhrman, Science 336, 555 (2012)
10 H. Chen, Q. Niu, and A. H. MacDonald, Phys. Rev. Lett. 112, 017205 (2014).
11 S. Nakatsuji, N. Kiyohara, and T. Higo, Nature 527, 212 (2015).
12 N. Kiyohara, T. Tomita, and S. Nakatsuji, Phys. Rev. Applied 5, 064009 (2016).
13 A. K. Nayak, J. E. Fischer, Y. Sun, B. Yan, J. Karel, A. C. Komarek, C. Shekhter, N. Kumar, S. Schnelle, J. Kübler, C. Felser and S. S. P. Parkin, Sci. Adv. 2, e1501870 (2016).
14 Y. Zhang, Y. Sun, H. Yang, J. Zelezný, S. S. P. Parkin, C. Felser and B. Yan, Phys. Rev. B 95, 075128 (2017).
15 W. Zhang, W. Han, S.-H. Yang, Y. Sun, Y. Zhang, B. Yan and S. S. P. Parkin, Sci. Adv. 2, e1600759 (2016).
16 T. Jungwirth, X. Marti, P. Wadley and J. Wunderlich, Nature Mano. 11, 231 (2016).
17 W. Nernst, Ann. Phys. 267, 760 (1887).
18 W.-L. Lee, S. Watauchi, V. L. Miller, R. J. Cava, and N. P. Ong, Phys. Rev. Lett. 93, 226601 (2004).
19 D. Xiao, Y. Yao, Z. Fang and Q. Niu, Phys. Rev. Lett. 97, 026603 (2006).
20 S.-g. Cheng, Y. Xing, Q.-f. Sun and X. C. Xie, Phys. Rev. B 78, 045302 (2008).
21 G. E. W. Bauer, E. Saitoh and B. J. van Wees, Nature Mater. 11, 391 (2012).
22 X. Li, L. Xu, L. Ding, J. Wang, M. Shen, X. Lu, Z. Zhu and K. Behnia, Phys. Rev. Lett. 119, 056601 (2017).
23 M. Ikhlas, T. Tomita, T. Koretsune, M.-T. Suzuki, D. Nishio-Hamane, R. Arita, Y. Otani and S. Nakatsuji, Nat. Phys. 13, 1085 (2017).
24 J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).
25 Y. Yao, K. Kleinman, A. H. MacDonald, J. Sinova, T. Jungwirth, D.-S. Wang, E.-G. Wang and Q. Niu, Phys. Rev. Lett. 92,037204 (2004).
26 G. Y. Guo, S. Murakami, T.-W. Chen, and N. Nagaosa, Phys. Rev. Lett. 100, 096401 (2008).
27 E. Kren and G. Kadar, Solid State Commun. 8, 1653 (1970).
28 P. E. Blöchl, Phys. Rev. B 50, 17953 (1994).
29 G. Kresse, J. Hafner, Phys. Rev. B 47, 558 (1993).
30 G. Kresse, J. Furthmüller, Phys. Rev. B 54, 11169 (1996).
31 O. Jepsen and O. K. Andersen, Solid State Commun. 9, 1763 (1971).
32 D. Xiao, M.-C. Chang, and Q. Niu, Rev. Mod. Phys. 82, 1959 (2010).
33 G. Y. Guo, Q. Niu, and N. Nagaosa, Phys. Rev. B 89, 214406 (2014).
34 B. Adolph, J. Furthmüller and F. Bechstedt, Phys. Rev. B 63, 125108 (2001).
35 G. Y. Guo, Y. Yao, and Q. Niu, Phys. Rev. Lett. 94,226601 (2005).
36 H.-R. Fuh and G. Y. Guo, Phys. Rev. B 84, 144427 (2011).
37 J.-C. Tung, H.-R. Fuh and G. Y. Guo, Phys. Rev. B 86, 024435 (2012).
38 J. Sticht, K.-H. Höck and J. Kübler, J. Phys.: Condens. Matter 1, 8155 (1989).
39 L. M. Sandratskii and J. Kübler, Phys. Rev. Lett. 76, 4963 (1996).
40 J. Kübler and C. Felser, Europhys. Lett. 108, 67001 (2014).
41 G. J. Zimmer and E. Kren, AIP Conf. Proc. 5, 513 (1971).
42 G. Kadar and E. Kren, Int. J. Magn. 1, 143 (1971).
43 S. Tomiyoshi, Y. Yamaguchi, T. Nagamiya, J. Magn. Magn. Mater. 31-34, 629 (1983).
44 T. Nagamiya, S. Tomiyoshi, Y. Yamaguchi, Solid State Commun. 42, 385 (1982).
45 W. Feng, G. Y. Guo, J. Zhou, Y. Yao and Q. Niu, Phys. Rev. B 92, 144426 (2015).
46 S. Meyer, Y.-T. Chen, S. Wimmer, M. Althammer, T. Wimmer, R. Schütz, S. Geprägs, H. Huebl, D. Ködderitzsch, H. Ebert, G. E. W. Bauer, R. Gross and S. T. B. Goennenwein, Nat. Mater. 16, 977 (2017).
47 H. Yang, Y. Sun, Y. Zhang, W.-J. Shi, S. S. P. Parkin and B. Yan, New J. Phys. 19, 015008 (2017).
48 J. Weischenberg, F. Freimuth, S. Blügel, and Y. Mokrousov, Phys. Rev. B 87, 060406 (2013).
49 J. P. Moore and R. S. Graves, J. Appl. Phys. 44, 1174 (1973).