Large Transverse and Longitudinal Magneto-Thermoelectric Effect in Polycrystalline Nodal-Line Semimetal Mg$_3$Bi$_2$

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Topological semimetals provide new opportunities for exploring novel thermoelectric phenomena, owing to their exotic and nontrivial electronic structure topology around the Fermi surface. Herein, the discovery of large transverse and longitudinal magneto-thermoelectric (MTE) effects in Mg$_3$Bi$_2$ is reported and predicted to be a type-II nodal-line semimetal in the absence of spin-orbit coupling (SOC). The maximum transverse power factor is 2182 $\mu$W m$^{-1}$K$^{-2}$ at 13.5 K and 6 Tesla. The longitudinal power factor reaches up to 3043 $\mu$W m$^{-1}$K$^{-2}$, which is 20 times higher than that in a zero-strength magnetic field and is also comparable to state-of-the-art MTE materials. By compensating the Mg loss in Mg-rich conditions for tuning the carrier concentration close to intrinsic state, the sample fabricated in this study exhibits a large linear non-saturating magnetoresistance of 940% under a field of 14 Tesla. Using density functional calculations, the authors attribute the underlying mechanism to the parent linear-dispersed nodal-line electronic structure without SOC and the anisotropic Fermi surface shape with SOC, highlighting the essential role of high carrier mobility and open electron orbits in the moment space. This work offers a new avenue toward highly efficient MTE materials through defect engineering in polycrystalline topological semimetals.

1. Introduction

Magneto-thermoelectric (MTE) effects include both transverse and longitudinal transport properties, depending on the directions of the magnetic field ($B$), temperature gradient ($\partial T/\partial r$), and voltage drop ($\partial V/\partial r$). Transverse-MTE is known as the Nernst effect,[1,2] wherein a nonzero $\partial V/\partial r$ occurs along the $\gamma$-axis if $\partial T/\partial r$ is along the $x$-axis and $B$ along the $z$-axis. Longitudinal-MTE constitutes the magneto-Seebeck effect,[1,4] where nonzero $\partial V/\partial r$ occurs along the $x$-axis if $\partial T/\partial r$ is along the $x$-axis and $B$ along the $z$-axis. The magnetic field plays a role of tuning the carrier transport, broadening the scope of the conventional thermoelectric effect for waste-heat harvesting and solid-state cooling.[5,6] Over the past years, significant progress has been made in the field of conventional thermoelectric materials through nanoscale engineering techniques, such as introducing various atomic defects, nano-inclusions, and grain boundaries.[8–10] By contrast, the MTE effect is susceptible to defects. Consequently, most previous studies have focused on the MTE effect in single crystals.[11,12] For instance, by applying a magnetic field, Chen et al. observed performance enhancement in the transverse power factor manipulated by the bipolar effect, which is the main Seebeck coefficient restriction in the power factor, and a transverse power factor of 400 $\mu$W cm$^{-1}$K$^{-2}$ was achieved at 30 K and 10 Tesla in single-crystal semimetal Mg$_3$Pb.[13] Compared with single-crystal materials, polycrystalline samples have obvious advantages in easily synthesizing large size samples, but challenges to tune the Fermi level towards the intrinsic state. As a result, the polycrystalline MTE materials have not yet gotten wide attention.

Fundamentally, MTE materials typically require an ultrahigh carrier mobility, electron–hole compensation, and a small Fermi surface.[2,14,15] Hence, topological semimetals are promising MTE materials because of their linear-dispersed low-energy excitation and special topological surface states.[14,16] Weyl semimetals and Dirac semimetals usually exhibit very high mobility owing to their massless Weyl and Dirac quasiparticles.[17–19] In addition, particle-hole-like symmetry usually exists in both Weyl and Dirac semimetals, in which the linear bands have led to almost equal concentrations of electron and hole carriers. In addition, the Fermi surface is tiny when the chemical potential is located around the charge-neutral band-crossing point. This could result in non-saturating magnetoresistance (MR) according to the electron–hole compensation mechanism based on the double carrier model,[20] as well as potentially a large longitudinal thermopower (see Part I, Supporting Information). Recently, large MTE effects were predicted theoretically in Weyl/Dirac semimetals,[18] and high thermoelectric performances...
were observed in experiments.\textsuperscript{[21-25]} Polycrystalline Weyl semimetal NbP shows a transverse thermopower of 90 $\mu$V K$^{-1}$ and a maximum transverse power factor of 3500 $\mu$W m$^{-1}$K$^{-2}$ at 136 K and 9 T, while its longitudinal power factor is only 850 $\mu$W m$^{-1}$K$^{-2}$ at 100 K and 9 Tesla.\textsuperscript{[24]} Wang et al. reported that the power factor of Dirac semimetal Cd$_3$As$_2$ single-crystal greatly increased under a perpendicular magnetic field, yielding power factor increase from 2150 to 4700 $\mu$W m$^{-1}$K$^{-2}$ at 300 K and 10 Tesla in single-crystal Pb$_{0.77}$Sn$_{0.23}$Se, and raised that gap inversion can change the sign of the Nernst signal.\textsuperscript{[24]} 

2. Results

2.1. Defects Engineering toward the Intrinsic Nodal-Line Semimetal Mg$_3$Bi$_2$

Mg$_3$Bi$_2$ has a crystalline structure with a trigonal lattice and space group $P\bar{3}m1$ (Figure S1a, Supporting Information).\textsuperscript{[35]} Bi is located in the interior of a single cell, while Mg usually has two positions: vertex Mg (Mg-I: 0, 0, 0) and interior Mg (Mg-II: 0.3333, 0.6667, 0.6300). The Mg at the vertex site can be easily lost during synthesis process, leading to the formation of Mg vacancy defects.\textsuperscript{[36]} Consequently, polycrystalline bulk Mg$_3$Bi$_2$ synthesized by high-temperature processes usually tends to present p-types, similar to the situation in Mg$_3$Sb$_2$.\textsuperscript{[37]} In addition, Mg vacancy could also scatter the carriers, resulting in limited mobility as reported previously for Mg$_3$Bi$_2$ single-crystal bulks.\textsuperscript{[33]}

To suppress Mg vacancies and optimize carrier mobility, a series of Mg$_3$Bi$_2$ samples with a nominal composition of Mg$_{x+y}$Bi$_2$ ($x = 0, 0.1, 0.2, 0.3, 0.4, \text{and} 0.5$) were successfully synthesized under different Mg compensations with nominal composition using mechanical alloying and spark plasma sintering (SPS) (Table S1, Supporting Information). Among the as-fabricated polycrystalline Mg$_3$Bi$_2$ samples [indexed as sample #1 ($x = 0$), #2 ($x = 0.1$), #3 ($x = 0.2$), #4 ($x = 0.3$), #5 ($x = 0.4$), and #6 ($x = 0.5$) with different Mg-rich nominal compositions], sample #5, that is, Mg$_{3.5}$Bi$_2$, is determined to be closest to the intrinsic state of the Mg$_3$Bi$_2$ nodal-line semimetal through Hall resistivity and thermal conductivity measurements (refer to Part II and Figures S1–S4, Supporting Information). The intrinsic state is a critical requirement for optimizing the carrier mobility and intrinsic Fermi surface shape to enhance the MTE effect.\textsuperscript{[38]} Through the double carrier model for Hall resistivity $\rho_{xy}^{(2)}$,\textsuperscript{[39]}

$$\rho_{xy} = \frac{1}{e} \left( \mu_{h} \mu_{e} - n_{h} n_{e} \right) + \mu_{h}^{2} \mu_{e}^{2} B^{2} (n_{h} - n_{e})$$

(1)

The carrier mobility of the obtained Mg$_3$Bi$_2$ sample in this work is calculated as $\mu_{c} = 4843$ cm$^2$V$^{-1}$s$^{-1}$ and $\mu_{h} = 1393$ cm$^2$V$^{-1}$s$^{-1}$, which is much higher than reported single-crystal bulk (450 cm$^2$V$^{-1}$s$^{-1}$) and single-crystal film Mg$_3$Bi$_2$ materials (120 cm$^2$V$^{-1}$s$^{-1}$) in previous studies.\textsuperscript{[13,14]}

2.2. Large Transverse and Longitudinal Magneto-Thermoelectric (MTE) Effect

Figure 1 shows the transverse-MTE and longitudinal-MTE properties of the as-fabricated polycrystalline Mg$_3$Bi$_2$ (sample #5) with a nominal composition of Mg$_{3.5}$Bi$_2$. To study the transverse-MTE properties, that is, Nernst effect of the Mg$_3$Bi$_2$ sample, we measured the transverse thermopower $S_{xy}$ (i.e., $\partial T/\partial x$ along $x$-axis, $\partial T/\partial y$ along $y$-axis, and $B$ along $z$-axis) at 1, 3, 6, 9, and 13 Tesla at temperatures range from 2 to 275 K. $S_{xy}$ increases with the increasing magnetic field and reaches a peak value of 127 $\mu$V K$^{-1}$ at 13 Tesla and 13.5 K (Figure 1a), which exceeds the previously reported values for polycrystalline NbP,\textsuperscript{[22]} and is comparable to that of single-crystal Pb$_{0.77}$Sn$_{0.23}$Se.
in the low magnetic field range.\cite{24} A more detailed comparison is presented in Figure S5, Supporting Information. The higher transverse thermopower, the higher Nernst coefficient, in accordance with $N_{xy} = S_{xy}/\mu_0 H$ (Figure S6, Supporting Information).\cite{40} The Nernst coefficient of the as-fabricated polycrystalline Mg$_3$Bi$_2$ gradually decreases with the increase of magnetic field, consistent with the behavior of other topological materials.\cite{41}

The temperature-dependent longitudinal thermopower was measured under different magnetic fields to examine the longitudinal-MTE properties (magneto-Seebeck effect). Figure 1b shows the longitudinal thermopower of the Mg$_3$Bi$_2$ sample at 0, 3, 6, 9, and 13 Tesla in a temperature range of 2 and 275 K, reaching a maximum value of 176 $\mu$V K$^{-1}$ at 15 K and 13 Tesla, which corresponds to 13 times enhancement. The longitudinal-MTE effect of Mg$_3$Bi$_2$ is also sensitive to the Mg-rich conditions (Figure S7a, Supporting Information), which is consistent with the behavior of other topological materials.\cite{41}

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The observed high and non-saturating longitudinal thermopower feature found in Mg$_3$Bi$_2$ illustrates that the large and non-saturating thermopower could also be extended to nodal-line semimetals. The transverse power factor $P_{xy}$ and longitudinal power factor $P_{xx}$ can be calculated by:\cite{22}

\begin{align}
P_{xy} &= S_{xy}^2 \sigma_{xx} \quad \text{(2a)} \\
P_{xx} &= S_{xx}^2 \sigma_{yy} \quad \text{(2b)}
\end{align}

The as-fabricated Mg$_3$Bi$_2$ is a polycrystalline material, and consequently, the electrical conductivity is isotropic; thus, $\sigma_{xx}$ should be equal to $\sigma_{yy}$. The calculated $P_{xy}$ and $P_{xx}$ values for different magnetic fields are plotted in Figures 1c and 1d, respectively. As the magnetic field strength increased, the transverse power factor $P_{xy}$ of Mg$_3$Bi$_2$ shows a peak at 6 Tesla, while the longitudinal power factor $P_{xx}$ exhibits unsaturated growth. The highest unsaturated $P_{xx}$ is 3043 $\mu$W m$^{-1}$K$^{-2}$ at 15 K under 13 Tesla, which is 20 times higher than the value at zero magnetic field strength. This value is also higher than that of most previously reported MTE materials, such as polycrystalline NbP (850 $\mu$W m$^{-1}$K$^{-2}$ at 100 K and 9 Tesla), polycrystalline Ag$_2$Se ($\approx$ 1250 $\mu$W m$^{-1}$K$^{-2}$ at 300 K and 5 Tesla), single-crystal FeGe$_2$ (625 $\mu$W m$^{-1}$K$^{-2}$ at 250 K and 9 Tesla), and single-crystal Cd$_3$As$_2$ (2500 $\mu$W m$^{-1}$K$^{-2}$ at 450 K and 7 Tesla).\cite{22,42-44} Besides, the highest $P_{xy}$ of 2182 $\mu$W m$^{-1}$K$^{-2}$ at 13.5K at 6 Tesla, obtained in the as-fabricated polycrystalline Mg$_3$Bi$_2$, is higher than polycrystalline Ag$_2$Se ($\approx$ 35 $\mu$W m$^{-1}$K$^{-2}$ at 300 K and 5 Tesla), polycrystalline Bi$_{77}$Sb$_{23}$ (540 $\mu$W m$^{-1}$K$^{-2}$ at 50 K and 5 Tesla), and comparable to single-crystal Pb$_{0.77}$Sn$_{0.23}$Se (2100 $\mu$W m$^{-1}$K$^{-2}$ at 300 K and 10 Tesla), single-crystal Re$_2$Si$_7$ ($\approx$ 2100 $\mu$W m$^{-1}$K$^{-2}$ at

Figure 1. Transverse- and longitudinal-MTE properties of polycrystalline Mg$_3$Bi$_2$. a) The transverse thermopower and b) longitudinal thermopower of Mg$_3$Bi$_2$ under different magnetic fields in a temperature range of 2 and 275 K. c) Changes in transverse power factor and d) longitudinal power factor of Mg$_3$Bi$_2$ with increasing magnetic field at 13.5 and 15 K, respectively.
550 K and 1.4 Tesla), and close to the value for polycrystalline NdP (3500 μW m⁻¹K⁻² at 150 K and 9 Tesla).

Furthermore, at low-temperature near 15 K, the MTE power factors of $P_{xx}$ and $P_{xy}$ are much higher than those of conventional thermoelectric materials (Figure S9, Supporting Information), demonstrating the advantages of MTE materials.

2.3. Large Magnetoresistance (MR) Effect

The key features of MTE materials with large transverse thermopower have been typically attributed to ultrahigh carrier mobility and electron–hole compensation, which are the exact conditions required for large MR. Owing to the presence of electrons and holes, topological semimetals usually exhibit very high MR, which is even not saturating at higher magnetic field strengths of tens of Tesla. Its electrical conductivity $\sigma$ can be significantly modulated under a magnetic field (Part III, Supporting Information), modifying MR and improving the longitudinal thermopower (Part I, Supporting Information). Therefore, the MR, which reflects the response of the electrical transport properties to a magnetic field, is closely related to the MTE effect. Figure 2a compares the MR of the as-fabricated polycrystalline Mg$_3$Bi$_2$ specimens with different nominal compositions of Mg$_{1+x}$Bi$_2$ ($x = 0, 0.1, 0.2, 0.3, 0.4, 0.5$) at 2 K and 7 Tesla. Detailed MR measurements are shown in Figure S10, Supporting Information. All the samples fabricated in this study have positive MR values between 2 and 300 K. Of note, the MR of sample #1 with a nominal composition of Mg$_{3.4}$Bi$_2$, shows a recording value of 940% at 2 K and 7 Tesla increases from 4% to 250%, 350%, 410%, 450%, and 413% as the nominal Mg-rich content $x$ increased from $x = 0$ to 0.1, 0.2, 0.3, 0.4, and 0.5, respectively. Sample #5, with a nominal composition of Mg$_{3.4}$Bi$_2$, shows a recording value of 940% at 2 K and 14 Tesla, which is two orders of magnitude higher than that of previously reported Mg$_3$Bi$_2$ single crystals. Notably, the MR is still unsaturated even at a magnetic field strength of up to 14 Tesla. Additionally, excessive Mg decreases the MR (sample #6, nominal composition of Mg$_{3.5}$Bi$_2$), further suggesting that sample #5 is closest to the intrinsic state of a semimetal.

2.4. Anisotropic MR

To understand the anomalous behavior of MR, we performed DFT electronic structure calculations as well as DFT-based transport calculations to simulate the variance of MR as a function of the external magnetic field along the $x$ and $z$ directions. Without considering SOC, the band crossing was close to the Fermi level, showing the type-II nature of the nodal line in Mg$_3$Bi$_2$ (Figure S11, Supporting Information). When including SOC, a small energy gap ($\approx 40$ meV, as shown in Figure 3a) at the nodal points is opened. The corresponding electrical conductivity tensor $\sigma$ of Mg$_3$Bi$_2$ was obtained by applying the following formula:

$$\sigma = \sum_n \sum_k \frac{e^2}{4\pi^2} \int \frac{dk}{\epsilon(k)} \epsilon(k) \nu_n(k) \bar{v}_n(k) \left( -\frac{\partial f}{\partial \epsilon} \right)_{\epsilon = \epsilon_n(k)} \quad (3)$$

where $e$ is the electron charge, $\epsilon_n(k)$ is the $n$th band energy at the momentum $k$ in the Brillouin zone with the corresponding relaxation time $\tau\epsilon_n(k)$, $\bar{v}_n(k)$ is the weighted average of the Fermi velocity $\nu_n(k)$, and $f$ is the Fermi distribution function of the equilibrium state. The total conductivity $\sigma$ is a summation of the individual band contribution $\sigma^{(n)}$; the MR, that is, the resistivity tensor $\rho$, can be obtained by inverting the conductivity tensor $\sigma$ (i.e., $\rho = \sigma^{-1}$). Equation (3) was calculated based on the tight-binding model by Wannier representation extracted from DFT wavefunctions (Part III, Supporting Information). In addition, a constant relaxation-time approximation was adopted. The weighted average group velocity $\bar{v}_n(k)$ reflects the nonlinear influence of the magnetic field on the electrical conductivity. A larger magnetic field involves more k points’ average (Equation (S8)), leading to saturating or non-saturating MR behavior.

The calculated transport results are shown in Figures 3c–f. The Fermi level was set to $E_F = 0.19$ eV (i.e., blue line in Figure 3a), corresponding to the as-fabricated sample.
#5 Mg$_3$Bi$_2$ obtained in this work, where the carrier mobility is optimal because of the change in the carrier effective mass (refer to Table S2 in Part IV, Supporting Information). This is also the band crossing point of the nodal line. First, an anisotropic MR was observed in hexagonal Mg$_3$Bi$_2$ when the magnetic field was applied along the $x$ axis (Figure 3c). The $z$-axis MR showed a nearly quadratic increase with the magnetic field, whereas the $y$-axis MR and $x$-axis MR were significantly smaller and rapidly saturated with $B$ (Figure 3c). We obtained a large and unsaturated $z$-axis MR of near 3000% at $B \tau = 14$(Tesla · ps) ($B // x$). On the other hand, when $B // z$ (Figure 3e), MR saturated in all three directions, approaching no more than 105%. Owing to the in-plane rotational symmetry under a perpendicular magnetic field, the MR along the $x$ and $y$ directions are degenerate.

### 2.5. Fermi Surface Topology

To explain the anisotropic MR behavior, we studied the Fermi surface topology of the Bloch electrons and the trajectories of the charge carriers driven by the Lorentz force. Figure 3b shows the Fermi-surface contours with $E_f = 0.19$ eV (blue line in Figure 3a). Based on the semiclassical scenario (refer to Equation (S9) in Part III, Supporting Information), the directions of the magnetic field $B$, Fermi velocity $v_n(k(f))$, and derivative of $k$ (i.e., $k$) are perpendicular to each other. Thus, the orbits of the Bloch electrons in the Brillouin zone are the cross-sections of the Fermi surface and a plane which is simultaneously normal to $B$ crossing the $k(f = 0)$ point. For $B // x$, the Fermi surface of the $k_z = 0$ plane is shown in the upper-right panel of Figure 3b. The hole orbits near the Gamma ($\Gamma$) point are closed.
circles, while the electron orbits are open, that is, extending throughout the Brillouin zone along the \( k_x \) direction, resulting in fewer electrons moving along the \( z \) direction compared to the zero magnetic field condition. As a result, with an increase in magnetic field strength along \( x \), the average velocity of the electrons along \( z \) decreases significantly (refer to Equation (S8) in Part III, Supporting Information), resulting in an increased resistivity \( \rho_{zz} \). To confirm this, we theoretically separated the contributions of the electrons and holes for resistivity \( \rho_{zz} \), as shown in Figure 3d. Electron resistivity exponentially increased with \( B \tau \) with a power factor of 1.82, while the hole contributions remained nearly unchanged upon magnetic field, consistent with the understandings of orbit topology.

For \( B/\tau \), the orbits of both the electrons and holes are closed (bottom right, Figure 3b), leading to the saturation properties of MR for all the directions. The separate contributions of the electrons and holes for \( \rho_{xx} \) shown in Figure 3f further confirm the closed-orbit nature of the Fermi surface. Considering that our experimental sample is polycrystalline, the total MR calculated by an average of all directions in a first-order approximation is consistent with our experimental results.

The above results imply that we could choose the optimal doping level in experiment to obtain large MR as well as MTE by designing the Fermi surface topology. Specifically, the Fermi level at \( E_F = 0.19 \) eV of Mg\(_3\)Bi\(_2\) is optimal for nonsaturated MR, where the high carrier mobility and open carrier orbits occur simultaneously. On the other hand, the nonsaturated MR effect will be suppressed as the Fermi level moves away from the optimal value, which is consistent with our MR measurements for various Mg doping levels (Figure 2a and Figure S12, Supporting Information). For example, when \( E_F = 0.15 \) eV, both the electron and hole orbits are almost closed (Figure S13a, Supporting Information), leading to a saturated MR for Mg\(_3\)Bi\(_2\) (Figures S12a and S12b, Supporting Information); when the Fermi level is further increased to 0.21 eV, more electron orbits around \( \Gamma \) are closed, not favorable for nonsaturated MR as well (Figures S12c, S12d, and S13c, Supporting Information). Of note, MR is small and saturated for the parent electronic structure without SOC at the band crossing point (Figure S14, Supporting Information). This indicates that the nodal-line semimetal with a tiny energy gap is a promising candidate system for realizing large MTE.

4. Experimental Section

Sample Preparation: The Mg\(_{1+x}\)Bi\(_2\) samples were synthesized through a combined approach of mechanical alloying and SPS. Magnesium turnings (Mg, 99.98%, Acros Organics) and bismuth shots (Bi, 99.999%, SN Plus) were weighed according to the composition of Mg\(_{1+x}\)Bi\(_2\) (\(0 \leq x \leq 0.5\)), and were loaded into a stainless-steel ball milling jar in a glove box under an Ar atmosphere with an oxygen level of <1 ppm. After ball milling for 10 h in a SPEX 8000M mixer, the ball-milled powders were loaded into a graphite die with an inner diameter of 15 mm, in the glove box. The graphite die with the loading powder was immediately sintered at 700 °C under a pressure of 50 MPa for 5 min via SPS (SPS-2111X, Fuji Electronic Industrial Co. LTD). The SPS bulks were ≈15 mm in diameter, with a thickness of ≈8 mm.

Sample Characterization: The phase purity of the product was measured by powder X-ray diffraction (XRD) on a Rigaku D/Max-2550 instrument (Cu \( K \alpha \) radiation, \( \lambda = 1.5418 \) Å, 18 kW). The temperature-dependent thermal conductivity was measured adiabatically using the thermal transport option (TTO) on a Quantum Design Physical Property Measurement System (PPMS 14 Tesla) with one-heater and two-thermometer configuration. With the same option, the transverse and longitudinal thermopower were simultaneously measured adiabatically. The authors mounted the sample with transverse voltage leads, which were purposefully offset by a distance \( X \) from each other so that the longitudinal (Seebeck) and transverse (Nernst) voltage could both be measured. The heat flowed from left to right, and the thermometers T-hot and T-cold were mounted on the left and right leads located on the lower side of the sample. The \( V_x \) and \( V_y \) leads measured the diagonal voltage component, and by measuring it as a function of the magnetic field in both the positive and negative fields, they could employ symmetry arguments to separate the longitudinal thermopower from the transverse thermopower. The longitudinal and Hall resistivities were measured using the electronic transport option (ETO) in Physical Property Measurement System (PPMS) using the standard four-probe method.

Calculation Methods: Electronic structure calculations were based on the DFT implemented in the Vienna ab initio simulation package (VASP),\(^{[55,56]}\) where the exchange-correlation potential was treated by generalized gradient approximation (CGA) of the Perdew–Burke–Ernzerhof (PBE) functional\(^{[57]}\) and the ionic potential was based on the projector augmented wave (PAW) method.\(^{[58,59]}\) Owing to the strong relativistic effect in Bismuth, SOC was also considered for the energy band dispersion calculations. The energy cutoff of the plane wave was set to 600 eV. For Brillouin zone sampling, a \( 19 \times 19 \times 9 \) \( \Gamma \) centered \( K \)-point mesh was used for the 5-atom unit cell for self-consistent calculations, and an \( 11 \times 11 \times 5 \) mesh was used for structure relaxation. The convergence criteria of the energy and force were set to \( 10^{-6} \) eV and 0.002 eV Å\(^{-1} \), respectively. The tight-binding model Hamiltonian adapted for the Wannier interpolation implemented in the WannierTools package\(^{[52,53]}\) (i.e., electrical conductivity calculation) was constructed by the Wannier90 software\(^{[60]}\) using the maximally localized Wannier function approach.\(^{[61–63]}\) The s, p orbits of Mg and p orbits of Bi were selected as the initial projectors for Wannier90 software.
defect engineering, Fermi surface topology, magnetoresistance, corresponding author upon reasonable request.

Data Availability Statement
The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords
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