Strain engineering of the magnetic multipole moments and anomalous Hall effect in pyrochlore iridate thin films

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The recent observation of the anomalous Hall effect (AHE) without notable magnetization in antiferromagnets has suggested that ferromagnetic ordering is not a necessary condition. Thus, recent theoretical studies have proposed that higher-rank magnetic multipoles formed by clusters of spins (cluster multipoles) can generate the AHE without magnetization. Despite such an intriguing proposal, controlling the unconventional AHE by inducing these cluster multipoles has not been investigated. Here, we demonstrate that strain can manipulate the hidden Berry curvature effect by inducing the higher-rank cluster multipoles in spin-orbit–coupled antiferromagnets. Observing the large AHE on fully strained antiferromagnetic Nd3Ir2O7 thin films, we prove that strain-induced cluster T1-octupoles are the only source of observed AHE. Our results provide a previously unidentified pathway for generating the unconventional AHE via strain-induced magnetic structures and establish a platform for exploring undiscovered topological phenomena via strain in correlated materials.

INTRODUCTION

The anomalous Hall effect (AHE) is a fundamental transport phenomenon that has been universally observed in time-reversal symmetry broken systems. AHE can arise from two different forms of mechanism (1): extrinsic mechanism, such as skew scattering or side jump due to magnetic impurities, and intrinsic mechanism originating from Berry curvature in momentum space. Since the fundamental topological properties of electronic wave functions are encoded in the Berry curvature, AHE is considered as a powerful tool for probing the topological properties of materials (2, 3). In addition to its fundamental interest, AHE can be applied for memory devices (4).

Conventionally, AHE has been observed mostly in itinerant ferromagnets. Its magnitude is known to be proportional to the magnetization (5), which is a measure of broken time-reversal symmetry. Recently, a large AHE has been unexpectedly found in noncollinear antiferromagnets, such as Mn3X (X = Sn, Ge) (6–8) and GdPtBi (9), which do not exhibit spontaneous magnetization. This unconventional response indicates that ferromagnetism is not a necessary condition for AHE and suggests a possible alternative origin of AHE. A recent theory proposed that higher-rank magnetic multipole (cluster multipole) moments formed from spin clusters in antiferromagnet can induce a nonzero AHE, beyond the conventional dipoles of ferromagnets (10). Subsequently, the anomalous Nernst (11) and magneto-optical Kerr effects (12) in Mn3Sn have also been attributed to its cluster octupoles. However, since antiferromagnets are not easily coupled to both magnetic and electric fields (13), it is very difficult to manipulate the higher-rank cluster multipoles. This imposes substantial limitations on controlled experiments on the cluster multipoles and associated AHE.

Here, we demonstrate that the strain can generate the AHE by inducing the higher-rank cluster multipoles, by using antiferromagnetic Nd3Ir2O7 (NIO) thin film. Further investigation reveals that biaxial strain on the pyrochlore lattice can modulate the spin structure and induce certain magnetic octupoles. The induced cluster octupoles can generate the net Berry curvature effect hidden in the bulk, leading to a finite AHE. We expect that our method could be widely applied to other spin-orbit–coupled topological magnets (10) and antiferromagnetic spintronics (4, 14).

RESULTS

Strain-induced cluster multipoles in a pyrochlore lattice

The NIO belongs to the pyrochlore iridates family, R3Ir2O7 (R, rare-earth ions). The members of the family are geometrically frustrated magnets with complex lattice structures. As shown in Fig. 1A, R3Ir2O7 is composed of linked tetrahedrons with R and Ir at each vertex. In R3Ir2O7, strong electron correlations and large spin-orbit coupling of Ir d electrons result in unique antiferromagnetic spin structures, called all-in-all-out (AIAO) ordering (15, 16). As shown in the circle in Fig. 1B, the spins in one tetrahedron point inward and those in the neighboring tetrahedron point outward. The Néel temperatures of the Ir and Nd sublattices of bulk NIO are TN ~ 30 K (15) and TNd ~ 15 K (17), respectively. This AIAO ordering breaks the time-reversal symmetry, allowing a nonzero Berry curvature distribution and generating correlated topological phases (18, 19) such as a Weyl semimetal.

However, since AIAO ordering preserves the cubic crystalline symmetry, the net Berry curvature effect vanishes when we integrate over the Brillouin zone (BZ). Unless the cubic crystalline symmetry is broken, AHE cannot be observed in this system. To break the

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cubic symmetry, a magnetic field was applied to pressured NIO single crystals (19) and Pr-doped bulk samples (20, 21). However, the spin structures modulated by the magnetic field are fragile and easily return once the magnetic field is turned off. Thus, a stable method to break the cubic symmetry is highly desirable; here, we choose a strain engineering approach and investigate the associated AHE.

As shown in Fig. 1B, the biaxial strain elongates the unit tetrahedra along the [111] direction. This will naturally break the cubic symmetry of the system. Since the deformation modulates magnetic anisotropy (22), the Ir spin directions should be changed. To systematically describe the change of spin direction, we adopted the cluster multipole theory. Since the conduction electrons come from Ir $d$ orbitals, we considered Ir sublattice only (16). In the cubic pyrochlore lattice, all spin ordering patterns can be classified into five different irreducible representations, carrying 12 distinct cluster multipoles (18). Among them, certain cluster multipoles that break the cubic symmetry are responsible for the AHE (see section S1).

In a bulk NIO, the AIAO ordering corresponds to a higher-rank magnetic multipole called the $A_2$-octupole (Fig. 1C). Since the $A_2$-octupole preserves the cubic symmetry, it cannot generate AHE. However, in a strained NIO (s-NIO), the AIAO spin structure becomes modulated under the strain. The resulting spin configuration is denoted by strained AIAO (s-AIAO), composed of a superposition of three kinds of cluster multipoles, namely, a dipole, an $A_2$-octupole, and a $T_1$-octupole ($\omega$). $M$ represents a ferromagnetic ordering, while $\omega$ represents an antiferromagnetic ordering other than AIAO. On the basis of symmetry analyses (see section S1 and table S1), we demonstrated that only the $T_1$-octupole can induce the AHE without magnetization.

**Characterizations of relaxed and fully s-NIO thin films**

To investigate the strain-induced magnetic multipole and associated AHE, we prepared two kinds of NIO thin films on the yttria-stabilized zirconia (YSZ) substrates: relaxed and fully strained films. The biaxial strain can arise from the lattice mismatch between the $R_2\text{Ir}_2\text{O}_7$ film and the YSZ substrate (see Fig. 1B) (23, 24). Since the lattice parameter of YSZ is smaller than those of NIO bulk, the NIO film should be compressively strained. We estimated the strain $\varepsilon$ ($\varepsilon = \frac{2a_{\text{YSZ}} - a_{\text{NIO}}}{a_{\text{NIO}}}$).
to be $-0.96\%$, where $a_{\text{NIO}}$ and $a_{\text{YSZ}}$ are lattice constants of bulk NIO (10.38 Å) and YSZ (5.14 Å), respectively. Despite the substantial past efforts (25–27), the in situ growth of high-quality $R_2\text{Ir}_2\text{O}_7$ thin film is notoriously difficult. Under the proper crystalline growth conditions for pyrochlore oxides (28), the corresponding $R_2\text{Ir}_2\text{O}_7$ phase forms extremely unstable because of the formation of a gaseous $\text{IrO}_3$ phase (29). To avoid this instability, many studies have used the “solid-phase epitaxy (SPE)” (25, 27) method, which involves the initial growth of amorphous $R_2\text{Ir}_2\text{O}_7$ films at a lower temperature ($T$) followed by ex situ thermal annealing in a sealed tube. Although SPE can provide a method for the growth of single-phase $R_2\text{Ir}_2\text{O}_7$ films, it usually produces relaxed films (25, 26). Therefore, we developed a previously unknown in situ film growth method, i.e., repeated rapid high-temperature synthesis epitaxy (RRHSE; see section S2 and Materials and Methods) (30).

The RRHSE method made us successfully grow the fully s-NIO films on YSZ (111) substrates. Figure 2A shows an x-ray diffraction $\theta$-2$\theta$ scan. The NIO (III) and YSZ (III) (l: integer) peaks can be seen, indicating epitaxial growth of NIO single phase. Particularly, the satellite peaks near the NIO (222) peaks are observed, which is commonly called “thickness fringes.” These interference peaks indicate the high quality of a sharp interface between film and substrate. Figure 2B shows x-ray reciprocal space mapping around the NIO (662) and YSZ (331) Bragg peaks of a 9-nm-thick NIO film. The lattice parameter of the (662)-plane, $d_{662}$, of bulk NIO is 1.19 Å, and the $d_{331}$ of YSZ is 1.18 Å. Note that the NIO (662) Bragg peak has the same $Q_x$ value as the YSZ (331) peak, demonstrating that our film becomes fully strained (~1% compressive strain) by the substrate.

Figure 2C shows a scanning transmission electron microscopy image that indicates the high quality of our film. The NIO pyrochlore phase is formed with few structural defects or disordered structures. Figure 2 (D and E) shows fast Fourier transform patterns from the selected areas in the film and substrate, respectively, marked in Fig. 2C. As demonstrated by the red dotted lines, the as-grown NIO film has the same inverse lattice constant as the YSZ substrate, which also confirms that our film is fully strained.

**Electronic structures of relaxed and fully s-NIO thin films**

We compared these fully s-NIO films grown by RRHSE with the relaxed NIO (r-NIO) films grown by the SPE (see section S3). The resistivity $\rho$ ($T$) curve of a 9-nm-thick s-NIO film exhibits a semimetallic behavior at most $T$. As shown in Fig. 3A, the s-NIO film has $\rho$ ($T$) an order of magnitude smaller than that of the r-NIO film. The $\rho$ ($T$) curve of an 80-nm-thick r-NIO film exhibits a metal-insulator transition around $\sim30$ K (black dashed line in Fig. 3A), in agreement with its bulk counterpart (17, 31). The strong upturn of the r-NIO film is due to its insulating nature below $T_{\text{N}} \approx 30$ K (17, 31). The $\rho$ ($T$) curve of the r-NIO film follows the Arrhenius plot (not shown here) in the low $T$ region, indicating a bandgap opening. In contrast, the $\rho$ ($T$) curve of the s-NIO film has a positive slope for most $T$ (orange line in Fig. 3A), suggesting that the film should be in a semimetallic state. Converting the resistivity into conductivity, the s-NIO film has $\sigma_{xx} \sim 1600$ ohms$^{-1}$ cm$^{-1}$ at 2 K. The tiny upturn below $\sim30$ K might arise from disorder effects.

To understand the corresponding electronic structure changes, we performed mean-field calculations using the Hubbard model (see section S4). The previous study shows that the most valence and conduction bands near the Fermi energy come mainly from Ir 5$d$ electrons (16). Our calculated electronic structure of the bulk (the r-NIO film in our case) explains its insulating nature. The energy gap opens with a value of about 13 meV (Fig. 3B), which agrees well with the bulk value (32). Under $1\%$ compressive strain, the valence and conduction bands move, which slightly increases the direct gap at most $k$ regions. However, some valence and conduction bands become crossed with Fermi level; thus, small electron and hole pockets develop near $L_{1,2,3,4}$ (Fig. 3C), creating a semimetallic state. These model calculations can explain why the s-NIO film has a much smaller $\rho$ ($T$) than the r-NIO film.

**Large AHE in fully s-NIO thin films**

Besides, the s-NIO film shows a much larger anomalous Hall conductivity (AHC) compared to the r-NIO film. Figure 3D shows the magnetic field ($H$)–dependent AHC $\sigma_{xy}^A(H)$ at 2 K, obtained after subtracting the ordinary Hall contribution from the total Hall conductivity (see Materials and Methods). The $\sigma_{xy}^A$ curves of s- and r-NIO films are displayed by the circles and the dashed line, respectively. The $\sigma_{xy}^A(H = -9$ T) values of the s- and r-NIO films are 2.4 and 0.2 ohms$^{-1}$ cm$^{-1}$, respectively. The spontaneous Hall conductivity (SHC) $\sigma_{xy}^A(H = 0)$ of the s-NIO films is 1.04 ohms$^{-1}$ cm$^{-1}$, which
is much larger than that of the r-NIO film. Note that the small AHC and SHC in the r-NIO film might be induced by the net magnetization of A12O domain walls (33). However, the large AHC and SHC in the s-NIO suggest that the net Berry curvature effect can be modulated by the strain.

To cross-check, we compared our magnetotransport property values with those of ferromagnets. For example, (Ga, Mn)As (34) and CuCr2Se4·Brx (35) typically exhibit SHC with σxy(H = 0 T) ~ 1 to 10 ohm−1 cm−1 and σxy(H = 0 T) ~ 1000 ohm−1 cm−1. These ferromagnets follow a scaling relationship σxy ∝ σxx that implies the intrinsic nature of the AHE (5). Since σxy and σxx values for the s-NIO film also fall on the same scaling curve (see section S5), we confirmed the enhanced AHC and SHC of our fully-s-NIO film as the net Berry curvature effect.

Accordingly, we calculated the Berry curvature effect on AHC from the band structure obtained from the mean-field calculations mentioned above (see section S4). AHC can be obtained by integrating the Berry curvature Ω_{xy}(k) throughout the whole BZ (5):

$$\sigma_{xy} = \frac{e^2}{h} \frac{d^3 k}{2\pi^2} \int \sum_{\alpha} f(\epsilon_{\alpha}(k)) - \mu \Omega_{[111]}(k)$$

where $f(\epsilon_{\alpha}(k))$ is the Fermi-Dirac distribution function and $\mu$ is the chemical potential. Figure 3E shows the Berry curvature $\Omega_{[111]}(k)$ of NIO along its high-symmetry lines with $H = 0$. Sizable $\Omega_{[111]}(k)$ at the $L_1, 2, 3, 4$ points in the BZ (Fig. 3F) exists for both the r- and s-NIO systems. The Berry curvature at each high-symmetry point for the r-NIO is somewhat larger than that for the 1% s-NIO. However, for the cubic r-NIO, $\sigma_{xy}$ vanishes since the integration of $\Omega_{[111]}(k)$ over the BZ cancels out. Generally, when twofold rotation symmetries $C_2$ about the $x$, $y$, or $z$ axis exist, $\Omega_{[111]}(k)$ is canceled by $\Omega_{[111]}(k)$. In the r-NIO, all three $C_2$ exist, so the net $\Omega_{[111]}(k)$ contribution becomes hidden (9). In contrast, for the trigonal s-NIO, the breaking of all $C_2$ symmetries draw out a finite net $\Omega_{[111]}(k)$ contribution. Thus, the biaxial strain can promote the net Berry curvature effect originally hidden in the bulk, generating the large AHE in the s-NIO films.

**Antihysteresis of AHC**

Another notable feature of s-NIO film is that its $\sigma_{xy}(H)$ curve shows an intriguing antihysteresis-like behavior, displayed in Fig. 3D. When we sweep the $H$-field from −9 to +9 T, a sign change occurs at an $H$ value of about −1 T (circles in Fig. 3D). Similar behavior is also observed when we reverse the $H$-field sweep from +9 to −9 T. This $H$-dependent sign change of the AHC differs from a typical hysteretic response of most ferroic materials, where the sign change occurs during the domain switch to the opposite direction. Although a similar antihysteresis-like behavior has been also reported in an earlier Hall conductivity study of an NIO single crystal under hydrostatic high pressure (21), its origin has not fully investigated yet.
To understand our antihysteresis-like $\sigma^{\text{Nd}}_{xy}(H)$ curve, we used a phenomenological model (see section S6). The model is composed of two tangent hyperbolic functions; one is hysteric (blue line) and the other is nonhysteretic (green line) (see Fig. 4A). Since the experimental data (orange circles) agree with the sum of two tangent hyperbolic functions (black solid line), the antihysteric curve can be explained by the two different origins of $\sigma^{\text{Nd}}_{xy}$. To obtain further insight, we measured $T$-dependent $\sigma^{\text{Nd}}_{xy}(H)$ curves of s-NIO film below 40 K. As shown in Fig. 4B, $\sigma^{\text{Nd}}_{xy}$ does not exist at 40 K, when the system is in a paramagnetic phase. As $T$ decreases, $\sigma^{\text{Nd}}_{xy}$ starts to emerge at ~30 K and becomes stronger thereafter. In 15 K < $T$ < 30 K, $\sigma^{\text{Nd}}_{xy}$ exhibits no hysteretic behavior. However, as $T$ decreases further below 15 K, $\sigma^{\text{Nd}}_{xy}$ starts to show the antihysteresis-like behavior. Figure 4B shows that all $T$-dependent $\sigma^{\text{Nd}}_{xy}$ curves are well matched with the sum of the nonhysteretic and hysteretic hyperbolic functions. Note that the bulk NIO has $T^{\text{Nd}}_{N} \sim 15$ K and $T^{\text{Nd}}_{h} \sim 30$ K (17), suggesting that the hysteretic and nonhysteretic responses are developed because of the magnetic orderings of Nd and Ir spins, respectively.

Figure 4C summarizes the results of the AHC fitting at $H = -9$ T with the $T^{\text{Nd}}_{N}$ and $T^{\text{Nd}}_{h}$ values, marked as the dotted lines. Note that, most transport in NIO occurs by Ir $d$ electrons near the Fermi level. This carrier transport can be affected by the spin ordering at the Ir and Nd sublattices. In Fig. 4C, the nonhysteretic component (green circles) starts to emerge below $T^{\text{Nd}}_{N}$, so it can be attributed to the Ir spin ordering, and we denote the nonhysteretic as $\sigma^{\text{Ir}}_{xy}$. On the other hand, the hysteretic component (blue circles) starts to emerge below $T^{\text{Nd}}_{h}$, so it can be attributed to the Nd spin ordering, and we denote the hysteretic as $\sigma^{\text{Nd}}_{xy}$. The nonhysteretic contribution of Ir is due to the absence of the Ir-AIAO domain switch through the smallness of Ir-AIAO coupling to the field. Meanwhile, the hysteretic contribution of Nd is due to the presence of the Ir-AIAO domain switch through $f$-$d$ exchange with either Nd-3OII or Nd-311O, which can be formed by large Nd moments under a [111] magnetic field (see section S6). This hysteretic behavior of $\sigma^{\text{Nd}}_{xy}$ leads to the finite SHC at zero field $\sigma^{\text{xy}}_{\text{Nd}}(H = 0)$ displayed as the red squares in Fig. 4C. Note that the SHC emerges below $T^{\text{Nd}}_{N}$.

**AHE from strain-induced $T_1$-octupoles**

To reveal the relation of AHE and cluster multipoles under strain, we should compare $M$ and $\sigma^{\text{Nd}}_{xy}$ values (see Fig. 1D). The $H$-dependent $M$ and $\sigma^{\text{Nd}}_{xy}$ hysteresis curves at 3 K are displayed in Fig. 5A, and associated $\sigma^{\text{Ir}}_{xy}$ and $\sigma^{\text{Nd}}_{xy}$ curves are shown in Fig. 5B. Figure 5A demonstrates that the conventional understanding of the SHC (5), i.e., $\sigma^{\text{Nd}}_{xy}(H = 0) \propto M(0)$, does not hold for the s-NIO film. Although the s-NIO film has a large SHC signal (orange circles) shown in Fig. 5A, it has no spontaneous $M$ at 3 K with $H = 0$ (purple squares) within the measurement error ($\pm 0.01 \mu_\text{B}$/NdIrO$_{3.5}$). As shown in Fig. 1D, the biaxial deformation of pyrochlore lattice can generate three kinds of multipoles, i.e., a dipole, an $A_2$-octupole, and a $T_1$-octupole. The dipole is crossed out because of the zero magnetization of our data, and the $A_2$-octupole is crossed out because of its zero contribution to AHC. Therefore, the strain-induced $T_1$-octupole should play important roles in generating the AHC without magnetization.

To elucidate how $T_1$-octupole emerges under the strain, we calculated the spin structure from the spin model. Since both Nd and Ir spins play important roles, we included the Heisenberg, Dzyaloshinskii-Moriya, anisotropic spin–exchange interactions between Ir spins (36), the $f$-$d$ exchange interaction between the Ir and Nd spins (17), and the Zeeman energy for both the Ir and Nd spins (for details, see section S7). On the basis of the calculated spin structure, we obtained the cluster multipoles (table S1 in section S1). Figure 5C shows the calculated dipole ($M$, green circles) and $T_1$-octupole ($\omega$, blue circles) as a function of the effective Zeeman energy $h$ in the r-NIO. According to our calculation, r-NIO does not have a finite $M$ or $\omega$ value for the Ir sublattice at $h = 0$. The zero values of $M$ and $\omega$ can explain the negligible SHC of the r-NIO film (see Fig. 3D). Figure 5D shows the calculated $M$ and $\omega$ of s-NIO, which are finite even for $h = 0$. Particularly, the hysteresis curve of $\omega$ looks similar to the $\sigma^{\text{Nd}}_{xy}$ curve in Fig. 5B. Therefore, we conclude that the large spontaneous $\omega$ that generate AHE can be induced by the strain in the s-NIO film.

**DISCUSSION**

Our work demonstrates that the strain-engineering of an antiferromagnet can generate the net Berry curvature effects by modulating its cluster multipoles. In particular, our findings highlight that the strain-induced $T_1$-octupole is closely connected with the topological properties of NIO. We can further extend this strain-engineering approach to search for the other novel topological phenomena in correlated magnets. For example, the strain engineering approach
line is the contribution of Ir spins, i.e., nonzero value of \( \sigma_{xy} \) becomes the origin of the SHC in our respectively. The strain-induced understand their fundamental mechanisms. 

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using the RRHSE method. This film growth method is a modi-

MATERIALS AND METHODS

Film growth and structural characterization

Fully s-NIO films were in situ grown on insulating YSZ substrates using the RRHSE method. This film growth method is a modified form of pulsed laser deposition, based on repeated short-term thermal annealing processes using an infrared laser. RRHSE consists of two key steps in one thermal cycle. During the first step, amorphous stoichiometric NIO and IrO\(_2\) layers were deposited by a KrF excimer laser (\( \lambda = 248 \) nm, 5 Hz) at \( T \approx 600^\circ\mathrm{C} \) with \( P_{\text{O}} = 50 \) mtorr. The additional IrO\(_2\) layer was deposited to compensate for the Ir loss that would unavoidably occur later during the synthesis process. During the second step, the pyrochlore phase is formed by rapidly raising \( T \) to 800\(^\circ\mathrm{C}\) (up to \( \sim 400^\circ\mathrm{C} \) min\(^{-1}\)). We must expose the sample to the high \( T \) for a period that is sufficiently long to syn-

thesize the pyrochlore phase but short enough to minimize the formation of IrO\(_3\). Last, we repeated these deposition and thermal synthesis processes until the desired film thickness was obtained. During the growth, the reflection high-energy electron diffraction pattern was monitored and the intensity of the oscillation was re-

After growth, NIO films were characterized by an x-ray dif-

fractometer (Bruker Corp.) and an atomic-resolution high-angle annular dark-field scanning transmission electron microscope (JEM-ARM200F; JEOL) equipped with an energy-dispersive x-ray spectrometer.

Transport and magnetic properties

Magnetotransport properties were measured via a standard four-

point probe method using a commercial physical property measurement system (PPMS, Quantum Design), which has a base \( T \) of 2 \( K \) and a maximum magnetic field of 9 \( T \). During the measurements, the current was applied along the [1-10] direction, and \( H \) was applied along the [111] direction. Magnetization data were obtained using a commercial superconducting quantum interference device magnetometer (MPMS, Quantum Design) with the magnetic field applied normal to the film.

The AHC value \( \sigma^A_{xy} \) can be obtained from the resistivity values, namely, \( \sigma^A_{xy}(H) = \frac{\rho^A_{xy}(H)}{\rho^A_{xx}(H)^2 + \rho^A_{yy}(H)^2} \) where \( \rho^A_{xy} \) is anomalous Hall resistiv-

ity and \( \rho_{xy} \) is longitudinal resistivity. To exclude the longitudinal contribution from the raw Hall resistivity data \( \rho_{xy} \), we used the antisymmetrization procedure (8, 9, 13). We separated the positive and negative field sweep branches and then antisymmetrized \( \rho_{xy} \) using \( \rho_{xy}^A(H) = \frac{\rho_{xy}(H) - \rho_{xy}(-H)}{2} \) and \( \rho_{xy}^A(H) = \frac{\rho_{xy}(H) + \rho_{xy}(-H)}{2} \). Note that \( \rho_{xy}^A(H) \) and \( \rho_{xy}^A(-H) \) denote positive field sweep (9 \( T \) to \(-9 \) \( T \)) and negative field sweep (\(-9 \) \( T \) to \(+9 \) \( T \)) branches, respectively. From \( \rho_{xy}^A(H) \) and \( \rho_{xy}^A(-H) \), we took out the linear part (ordinary Hall resistivity) to determine \( \rho^A_{xy} \).

Self-consistent mean-field Hubbard model

We developed the Hubbard model for the s-NIO thin film under the magnetic field and acquired the ground state and electronic structure by the self-consistent mean-field method. We adopted \( 24 \times 24 \times 24 \) and \( 32 \times 32 \times 32 \) \( k \)-point mesh and found that the re-

REFERENCES AND NOTES


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logical insulator (18), and line-node semimetal (19, 21) by properly modifying their magnetic structure. In this perspective, we believe that our strain study on NIO could provide a cornerstone to discov-
ear strain-engineered novel topological phenomena in oxides and to understand their fundamental mechanisms.

SUPPLEMENTARY MATERIALS

Supplementary material for this article is available at http://advances.sciencemag.org/cgi/content/full/6/29/eabb1539/DC1

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