Nanomechanical Characterization of an Antiferromagnetic Topological Insulator

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cite this: Nano Lett. 2025, 25, 973−980

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ABSTRACT: The antiferromagnetic topological insulator MnBi$_2$Te$_4$ (MBT) exhibits an ideal platform for investigating unique topological and magnetic properties. While the transport characteristics of magnetic phase transitions in the MBT materials have been extensively studied, the understanding of their mechanical properties and magneto-mechanical coupling remains limited. Here, we utilize nanoelectromechanical systems to probe the intrinsic magnetism in MBT thin flakes through magnetostrictive coupling. By analyzing the mechanical resonance signatures, we explore the magnetic phase transitions from antiferromagnetic (AFM) to canted antiferromagnetic (CAF) to ferromagnetic (FM) phases as a function of magnetic field. Our results reveal the spin-flop transitions in MBT, characterized by frequency shifts in the mechanical resonance. To establish a correlation between the frequency shifts and the spin-canting states, we employ a magnetostrictive model to extract the magnetostrictive coefficients. Our study demonstrates a valuable approach using nanoelectromechanical systems to investigate magnetic phase transitions, magnetization, and magnetoelastic properties in antiferromagnetic topological insulators.

KEYWORDS: Antiferromagnetic topological insulator, Nanoelectromechanical resonator, Magnetostriction, Spin-flop, Magnetic phase transition

Nanoelectromechanical systems (NEMS) have found widespread applications in nano filtering, ultrahigh sensitivity mass/force/pressure sensing, and molecular detection. NEMS based on graphene and 2D materials have been extensively studied for their high-performance characteristics, including ultralow mass density, exceptional mechanical flexibility, and stiffnesses. These 2D NEMS offer new opportunities for controlling mechanical, electrical, and optical properties across various degrees of freedom. For instance, they have been investigated for their optical properties and charge density wave transitions in transition-metal dichalcogenides, as well as for magnetic phase transitions in antiferromagnetic and ferromagnetic materials. Recently, researchers have leveraged field-induced magnetostriiction in magnetic 2D materials to achieve new control of magnetic and mechanical coupling in NEMS.

Another intriguing material in this field is the intrinsic magnetic topological insulator MnBi$_2$Te$_4$ (MBT), where spins are coupled in the ferromagnetic (FM) state, while interlayer coupling is antiferromagnetic (AFM). As an antiferromagnetic topological insulator, the MBT material family provides an excellent platform for studying new electronic and magnetic couplings with mechanical motion. The introduction of magnetism in the MBT leads to the emergence of exotic phenomena, including the quantum anomalous Hall effect, axion insulator state, and layer Hall effect. The band structures of the MBT compounds have been extensively studied using angle-resolved photoemission spectroscopy (ARPES), revealing that MBT is a heavily electron-doped compound with the Fermi level residing in the conduction band. Recent investigations using first-principles calculations, ARPES and transport measurements have demonstrated that the Fermi level of Mn-(Bi$_{1−x}$Sb)$_x$Te$_4$ can be tuned from the conduction band to the valence band by varying the Sb concentration.

The study of spin–lattice coupling in magnetic topological insulators has the potential to enable the detection, control and modification of spin states and magnetic structures. Previous research on MBT films has underscored the importance of magnon–phonon interactions and substrate effects in magnetic phase transitions, as evidenced by Raman spectroscopy measurements. Additionally, nanomechanical strain can be employed to detect magnetic states and their coupling with mechanical degrees of freedom. In this study, we focus on the exchange magnetostriction effect in Mn(Bi$_{0.8}$Sb$_{0.2}$)$_2$Te$_4$ (MBST) films by constructing a NEM resonator device structure. This device design, featuring a suspended membrane geometry, eliminates interaction between the sample and the substrates, allowing for cleaner manifestations of phase transitions.

Received: August 23, 2024
Revised: January 6, 2025
Accepted: January 8, 2025
Published: January 13, 2025
transitions. The exchange magnetostriction in the antiferromagnetic topological insulator MBST responds to changes in the magnetization of the Mn layer, inducing magnetostrictive strain in the film. This strain, induced by the magnetostrictive effect, is reflected in changes in the resonance frequency ($f_{\text{res}}$) of the NEM resonator. By monitoring shifts in $f_{\text{res}}$, we can distinguish different magnetic states and gain insight into the transition between them, thereby enhancing our understanding of spin-lattice coupling. To further support these findings, we determine the magnetoelastic energy parameters from magnetic field dependent $f_{\text{res}}$ measurements, which are corroborated by density functional theory (DFT) calculations.

The MBST NEM resonator devices were prepared following these steps: (i) bottom gate gold electrodes (30 nm) were photolithographically patterned on a highly resistive silicon wafer (600 μm); (ii) a SiO$_2$ layer (300 nm) was deposited using plasma-enhanced chemical vapor deposition; (iii) source and drain gold leads (25 nm) were patterned and deposited as in (i); (iv) a circular hole was etched down to the bottom gate electrode via a dry reactive-ion etching process; and (v) MBST flakes were exfoliated and transferred onto the prepatterened gold leads over the circular hole using a micromanipulator transfer stage. Figure 1a displays an optical image of a representative MBST NEM resonator device, consisting of an MBST flake with a thickness of about 30 nm, suspended over a hole with a radius of 4 μm. The schematic in Figure 1a illustrates the side view of the device structure, where the MBST flake and the underneath gold gate electrode form a parallel capacitor structure with vacuum as the dielectric. The two-terminal resistance of the MBST flake typically falls within the range of a few kΩ at room temperature.

Our transduction technique employs a high-frequency electrical circuit to actuate and detect the mechanical resonances in the MBST resonator device. A DC voltage applied to the gate electrode induces static tension and displacement in the MBST flake while the AC voltage is used to modulate the displacement. This alters the capacitance between the MBST flake and the gate electrode, which gives rise to a large capacitive contribution to the transmission on resonance.

The radio frequency (RF) measurements were conducted in a variable temperature insert at a base temperature of 1.5 K. Figure 1b illustrates the circuit diagram of the RF measurement setup. The mechanical vibrations were driven by an RF signal output from a vector network analyzer (VNA). This RF signal was coupled to a DC gate voltage through a bias tee, and the transmitted RF signal was decoupled using a second bias tee before being fed back to the VNA. The fundamental resonance mode of the MBST membrane was fitted to a Fano line shape with a peak frequency of about 32.7 MHz, exhibiting a quality factor ($Q$) exceeding 5000 (Supporting Information, Figure S1). This $Q$-value is comparable to those observed in other 2D magnet resonators and is similar to high-quality resonator made from graphene and WSe$_2$. Figure 1c presents a color plot of the RF transmission ($S_{21}$) as a function of frequency and gate voltage. The gate voltage ($V_g$) generates an electrostatic force that induce mechanical tension in the MBST membrane, shifting its resonance frequencies ($f_{\text{res}}$). The $f_{\text{res}}$ decreases to a minimum at $V_g \sim \pm 80$ V due to capacitive softening and then increases with a further increase in $V_g$ due to gate-induced stiffening, similar to other NEMS. The gate-dependent $f_{\text{res}}$ were fitted using a continuum mechanics model for a fully clamped membrane, as discussed
Magnetostrictive Parameters Obtained from DFT Calculations and Fitting to the RF Experimental Data for the MBST NEM Resonator

| Experiment | DFT |
|------------|-----|
| Mass density (kg/m³) | 7360 |
| Young’s modulus, E (GPa) | 84.374 |
| Poisson’s ratio, ν₀ | 0.212 |
| Built-in strain, ε₀ (%) | 0.83 |
| Built-in-stress, σ₀ (N/m³) | 88.24 |
| Magnetostrictive coefficients (meV): A₁₆ₓₓ | 9 |
| Aₓₓ | 0.6 |

on these parameters, we estimate a built-in strain ε₀ ≈ 0.83% in the MBST NEM resonator device. The relatively large ε₀ compared to other resonator systems, consistent with its “W”-shaped f(res)(Vtg) curve (Figure 1c), similar to high ε₀ graphene and MoS₂ based resonators.

Next, we investigate the effect of magnetic field on the f(res) for the MBST NEMS device. Due to the weak interlayer antiferromagnetic coupling, MBST device undergoes magnetic transitions under a perpendicular magnetic field. Figure 1d presents a color plot of S₂₁ as a function of frequency and magnetic field, with Vtg fixed at 70 V. We observe two distinct transitions in the magnetic field. The first transition is characterized by a jump in f(res) at around 3.7 T, while the second transition occurs at around 8 T, where the f(res) saturates with increasing magnetic field. These observed transitions in f(res) align with the magnetic phase transitions reported in previous studies on MBST.

Specifically, the first transition corresponds to a spin-flop process from AFM to the canted antiferromagnetic (CAFNM) phase, while the second transition corresponds to the transition from CAFM to the FM phase. Consistently, we have observed similar results in all of the fabricated MBST resonator devices that have been measured thus far (see Supporting Information 8, Figure S6 for additional data).

To further verify the field-induced magnetic phase transitions, we performed magnetotransport measurements on MBST devices. MBST flakes of similar thickness were fabricated into Hall bar devices using a standard electron beam lithography, with a Cr/Au contact electrode deposited in a thickness of 10/60 nm. The top gate was made by transferring hBN and graphene layers to serve as the dielectric and gate electrode, respectively, onto the Hall bar devices. Figures 2a and b show the gate and magnetic field dependent Rxx and Ryx for a 30 nm MBST Hall bar device (Figure 2d, inset). Line cuts of Rxx and Ryx were taken at different temperatures in the two distinct Hall signal regions: Vtg of +7.8 V (hole carrier) and +16.5 V (charge neutrality), as shown in Figures 2c–f. The discontinuous vertical steps observed in the Rxx color map at ±2.8 T are assigned to the spin-flop transition field (Hsf), which corresponds to the transition from AFM to CAFM states. Similarly, the second turning point in the Ryx curves indicates the saturation field (Hs), corresponding to the transition from CAFM to FM states. As temperature increases, the kink observed in Rxx diminishes and eventually disappears at 25 K, which is consistent with the Néel temperature Tᵅ of 23 K of the MBST. The blue and red arrows in Figures 2c–f track the evolution of H₁ and H₂ with temperature for the two carrier densities, respectively (refer to Supporting Information 6, Figure S4 for the full data set). Notably, the magnetotransport analyses indicate that H₁ and H₂ are nearly independent of the gate voltages, thereby excluding the possibility of carrier density modulated magnetic transitions in MBST.

Our NEM resonator devices demonstrate a clear relationship between the f(res) and the magnetic transitions. In Figures 3a–e, we present the magnetic field dependent S₂₁ measurements for the MBST resonator device at various temperatures. The

Figure 2. MBST Hall bar device. Color plots of (a) Rxx and (b) Ryx as functions of magnetic field and gate voltage for a 30 nm thick MBST flake. The data were taken at a temperature of 2 K. The blue and red horizontal arrows point to the top-gate voltages where the line cuts are taken. Plots of (c) Rxx and (d) Ryx as a function magnetic field taken at different temperatures with the top-gate voltage fixed to +7.8 V. Inset in (d) is the optical image of the MBST device. Plots of (e) Rxx and (f) Ryx as a function magnetic field taken at different temperatures with the top-gate voltage fixed to +16.5 V. The Rxx and Ryx line profiles are symmetrized and antisymmetrized, respectively. Vertical arrows in (c,e) and (d,f) point to the H₁ and H₂, respectively, at different temperatures.
disappearance of the transitions beyond the Neel temperature $T_N \sim 23 K$ confirms the correlation between $f_{\text{res}}$ and the magnetic transitions. Similar to our transport analysis, both $H_1$ and $H_2$ exhibit suppression with increasing temperature, albeit at different rates. The evolution of $H_1$ and $H_2$ with temperature below $T_N$, based on the change in $f_{\text{res}}$, is summarized in Supporting Information S5, Figure S3. At 25 K, we observe a monotonic increase in $f_{\text{res}}$ with the magnetic field, which is characteristic of a paramagnetic (PM) state. Notably, even at 10 K, $f_{\text{res}}$ is no longer saturates at high field; instead, it increases linearly with the magnetic field beyond $H_2$. The positive slope in $f_{\text{res}}$ follows a similar trend to the magnetic field dependent $f_{\text{res}}$ observed at 25 K. This indicates that the magnetic field does not prolong the FM state at higher temperature, consistent with observations from magnetic force microscopy. In contrast, the magnetic field dependent $f_{\text{res}}$ exhibits consistent behavior in the AFM and CAFM phases at different temperatures, indicating a robust AFM ground state in the MBST. At higher temperatures, the PM phase dominates the high magnetic field regime, while the CAFM phase is nearly suppressed. By extracting the $f_{\text{res}}$ data, we construct a magnetic phase diagram that incorporates the dependence on magnetic field and temperature, as shown in Figures 3a–e. Figure 3f presents a 2D color plot of the normalized resonance frequency, $f_{\text{res}}(B)/f_{\text{res}}(0)$, as a function of the magnetic field and temperature. The three magnetic phases, viz., AFM, CAFM, and FM states, are indicated for $T < T_N$, while the PM phase emerges at high temperature ($T > T_N$). The strong dependence of $f_{\text{res}}$ on both magnetic field and temperature provides robust support for the magnetic phase transition picture in the MBST sample.

The dependence of $f_{\text{res}}$ on the magnetic field indicates a magnetostrictive resonance. The mechanical resonance is correlated with the internal magnetic order, which changes with the external magnetic field. The $f_{\text{res}}$ reveals an abrupt change of about 0.32%, or equivalent to a $\Delta f_{\text{res}}$ of 105 kHz, around the $H_1$ at the base temperature. Beyond the spin-flop transition ($H > H_1$), the $f_{\text{res}}$ changes gradually with the magnetic field, eventually saturating at $H_2$. This behavior in CAFM state is absent in other 2D AFM materials, such as CrI$_3$ and CrOCl, indicating a correlation between $\Delta f_{\text{res}}$ and the canting angle of the spins. To quantify the spin–lattice coupling, we employ the magnetostriction model to fit our experimental data. According to this model, the shift in $f_{\text{res}}$ with the magnetic state results from the competition between internal magnetic energy and elastic energy. The free energies per unit area for a freestanding membrane in the AFM, CAFM, and FM states in the zero-temperature limit can be expressed as

**AFM state:**

$$F_{\text{AFM}} = nE_0 + (n - 1)J_{\perp}$$

**CAFM state:**

$$F_{\text{CAFM}} = nE_0 + (n - 1)J_{\perp} \cos \theta + \frac{1}{2}nK_\text{eff} \sin^2 \theta$$

**FM state:**

$$F_{\text{FM}} = nE_0 - (n - 1)J_{\perp} - \mu_0 \mu_0 \left( H_z - \frac{M_0}{t} \right)$$

where $\theta$ is the canting angle of the spin of Mn atoms, $n$ is the number of Mn layers, $J_{\perp}$ is the interlayer exchange in units of energy per unit area, and $K_\text{eff}$ is the anisotropy in units of energy per unit area. The total energy of the MBST membrane is thus the sum of the free energy of the membrane, the elastic energy and the boundary energy of the fully clamped drum. The elastic energy and the boundary energy of the membrane per unit area can be expressed as $U_\text{el} = \frac{1}{2} \sigma_0 \epsilon$ and $U_\text{b} = -\sigma_0 \epsilon$, respectively.

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**Figure 3.** Temperature dependence of magnetic phase transition probed by resonance frequency. Color plots of RF transmission signal $S_{11}$ as functions of driving frequency and magnetic field at a fixed gate voltage of +85 V at different temperatures of (a) 1.5 K, (b) 10 K, (c) 15 K, (d) 20 K, and (e) 25 K. (f) Magnetic phase diagram derived from the $f_{\text{res}}$. Color plot of $f_{\text{res}}(B)/f_{\text{res}}(0)$ as functions of magnetic field and temperature. The different magnetic phases of PM, AFM, CAFM, and FM states are labeled in the phase diagram.
respectively, where \( \epsilon \) is the strain and \( \sigma_0 \) is the built-in stress. By taking the derivative of the total energy with respect to strain and setting this derivative equation to zero to minimize total energy, we can derive the frequency changes between AFM state, cAFM state, and FM state as a function of the magnetostrictive coefficients and the spin canting angle. Using unit cell area \( A_u \approx 0.16 \text{ nm}^2 \) and \( n = 31 \text{ Mn layers} \) corresponding to a reasonable estimate for the thickness (42 nm) of the sample, we obtain one magnetostrictive coefficient: \( \frac{\partial \mu}{\partial \epsilon} A_u \approx 9 \text{ meV} \). By comparing the fractional change of \( f_{\text{res}} \) in the canted AFM state and AFM state, we obtain the other magnetostrictive coefficient: \( \frac{\partial K_{\text{eff}}}{\partial \epsilon} A_u \approx 0.6 \text{ meV} \) (Supporting Information 9). Using the values of the two magnetostrictive coefficients obtained above, we can fit the \( f_{\text{res}} \) as a dependence of magnetization. Figure 4a illustrates the correspondence between \( f_{\text{res}} \) and the absolute value of magnetization for the MBST as a function of the magnetic field. At low magnetic fields, the magnetization is almost zero. As the magnetic field approaches \( H_s \), there is a dramatic increase in magnetization. The magnetization increases monotonically with the magnetic field in the CAFM state and ultimately saturates in the FM state. The strong consistency between the \( f_{\text{res}} \)-correlated magnetization and the literature\(^{27,34,43} \) demonstrates the sensitivity of mechanical detection to magnetic states and their transitions.

To supplement the experimental results, we employ the DFT calculations to study the stability of the magnetic phases and to determine theoretical estimates for the magnetoelastic coefficients. Figure 4b plots the relative magnetic energy, \( \Delta E_\theta(\theta) \), versus the spin alignment angle for a two septuple layer MnBi\(_{0.9}\)Sb\(_{0.7}\)Te\(_4\) under the different external magnetic fields. The relative energy, \( \Delta E(\theta) \), for the AFM and FM configurations is obtained by manipulating the spin angle adjacent to the nearest spin layer, \( \theta \), as illustrated in the atomic lattice structures included in Figure 4b. The effect of the external magnetic field is incorporated by adding an energy gain term as \( -\mu_B \left( \frac{m_1 + m_2(\theta)}{2} \right) B \), where indexes 1 and 2 refer to the top and bottom septuple layer, respectively. At 0 T, the relative magnetic energy is minimized in the AFM ground state. As the external magnetic field increases, the energy of the spins aligned with the external field decreases, as indicated by the dotted colored lines in Figure 4b. Above the critical field \( (B_z = 3.509 \text{ T}, \text{ green line}) \), the relative magnetic energy of the FM state becomes negative, indicating that the FM state becomes energetically favorable compared to the AFM state. Subsequently, we show the magnetostriction effect due to in-plane tensile strain \( (\epsilon > 0) \) applied to the MBST system using DFT calculations. The changes in strain of the interlayer exchange coupling and magnetic anisotropic energies are obtained by

\[
\frac{\partial \epsilon}{\partial \epsilon} E_{\text{FM}} - E_{\text{AFM}}
\]

\[
\frac{\partial K_{\text{eff}}}{\partial \epsilon} = \frac{\partial}{\partial \epsilon} (E_{\text{FM},\epsilon} - E_{\text{AFM},\epsilon})
\]

where \( E_{\text{FM},\epsilon} \), \( E_{\text{AFM},\epsilon} \), and \( E_{\text{AFM}_x} \) denote the total energies of FM, \( x \)-directed AFM, and \( z \)-directed AFM phases. Increasing in-plane strain reduces the interlayer distance due to the Poisson ratio, resulting in a stronger interlayer exchange coupling. Using the built-in strain of 0.83% estimated from the experiments, we obtain the derivative of exchange and anisotropy with respect to strain for the MBST as \( \frac{\partial \epsilon}{\partial \epsilon} \approx 2.8 \text{ meV} \) and \( \frac{\partial K_{\text{eff}}}{\partial \epsilon} \approx 0.2 \text{ meV} \) (Supporting Information 10, Figure S7). The experimental and theoretical results for the two magnetostrictive coefficients are fairly consistent, with the interlayer exchange coupling in the few meV range and the anisotropy energy being 1 order of magnitude smaller. These magnetostrictive coefficients are also comparable to those found in other 2D antiferromagnets, such as CrI\(_3\)\(^{18} \) and CrOCl\(_3\)\(^{38} \).

In summary, we have observed an exchange magnetostriction effect in the antiferromagnetic topological insulator MBST. We studied the mechanical properties of MBST NEM resonator and obtained key mechanical parameters, such as the elastic modulus, built-in strain, and Q-factor. The resonance frequency was highly responsive to changes in the external magnetic field, indicating the presence of magneto–mechanical coupling in MBST. The magnetostrictive behavior of the suspended MBST film provided insights into different magnetic states within the magnetic phase diagrams. We developed a modified magnetostrictive model that accurately describes the spin flop transition in the CAFM state of MBST, respectively.
allowing us to extract the magnetization as a function of the magnetic field from the mechanical resonance measurements. Our results provide quantitative evidence for the correlation between intrinsic magnetic ordering and resonance frequency in MBST. Additionally, we quantified the exchange and anisotropy energies associated with strain using the magnetostriction model. Overall, our findings demonstrate the potential of the MBST-based NEM resonator structure as a new platform for exploring the inherent magnetism of MBT family materials.

**METHODS**

**Crystal Growth.** Bulk crystals of Mn$(\text{Bi}_1-x\text{Sb}_x)$$_2\text{Te}_4$ were synthesized using the Te-flux method. The manganese powder, bismuth shot, antimony shot, and tellurium lumps with a molar ratio of $1:5(1-x):5x:16$ were loaded in an alumina crucible and sealed in a quartz tube under a high vacuum. The mixture was heated to 900 °C for 12 h to promote the homogeneous melting and slowly cooled down to a temperature window of 590 to 630 °C at a rate of 1.5 °C/h. The plate-like single crystals can be obtained after removing the excess Bi–Te flux by centrifugation.

**DFT Calculations.** The first-principles calculations are performed within the framework of density functional theory (DFT) by Vienna an-iniito calculation package (VASP) in Perdew–Burke–Ernzerhof-type (PBE) generalized gradient approximation (GGA). To address the electron correlation due to the Mn 3d orbitals, we include a Hubbard $U–J$ parameter 4 eV. The energy cutoff for the plane-wave basis is set to 450 eV, and K-point sampling is done using a $12 \times 12 \times 2$ Monkhorst–Pack grid. All the crystal structures are fully relaxed until the atomic forces are below 1e$^{-2}$ eV/Å. vdW correction is included by the DFT-D3 method to better describe the interlayer dispersion forces.

**ASSOCIATED CONTENT**

**Supporting Information**
The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.nanolett.4c04086.

Additional experimental details, DFT calculations, magnetotransport and resonance frequency data, and continuum mechanics model and exchange magnetostriction model (PDF)

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**Authors Contributions**

S.W.L. performed the measurements, analyzed the data, and cowrote the manuscript under the supervision of V.V.D.; S.K.C. helped with sample preparation and performed the transport measurements under the supervision of K.L.W.; D.K. performed DFT calculations under the supervision of F.L.; A.V. helped with measurements; R.K. fabricated the substrates; S.H.L. grew and characterized the crystal under the supervision of Z.Q.M.; all authors viewed and commented on the manuscript; and V.V.D. supervised the whole project.

**Notes**

The authors declare no competing financial interest.

**ACKNOWLEDGMENTS**

This material is based upon work supported by the National Science Foundation of the Quantum Leap Big Idea under Grant No. 1936383. K.L.W. acknowledges support from the U.S. Army Research Office MURI program under Grants No. W911NF-20-2-0166 and No. W911NF-16-1-0472. S.K.C. acknowledges support from the Beijing Natural Science Foundation under Grant No. IS23022. The financial support for sample preparation was provided by the National Science Foundation through the Penn State 2D Crystal Consortium–Materials Innovation Platform (2DCC-MIP) under NSF cooperative agreement DMR-2039351.

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Nano Lett. 2025, 25, 973–980