Spin-dependent scattering induced negative magnetoresistance in topological insulator Bi$_2$Te$_3$ nanowires

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Studies of negative magnetoresistance in novel materials have recently been in the forefront of spintronic research. Here, we report an experimental observation of the temperature dependent negative magnetoresistance in Bi$_2$Te$_3$ topological insulator (TI) nanowires at ultralow temperatures (20 mK). We find a crossover from negative to positive magnetoresistance while increasing temperature under longitudinal magnetic field. We observe a large negative magnetoresistance which reaches $-22\%$ at 8 T. The interplay between negative and positive magnetoresistance can be understood in terms of the competition between dephasing and spin-orbit scattering time scales. Based on the first-principles calculations within a density functional theory framework, we demonstrate that disorder (substitutional) by Ga$^+$ ion milling process, which is used to fabricate nanowires, induces local magnetic moments in Bi$_2$Te$_3$ crystal that can lead to spin-dependent scattering of surface and bulk electrons. These experimental findings show a significant advance in the nanoscale spintronics applications based on longitudinal magnetoresistance in TIs. Our experimental results of large negative longitudinal magnetoresistance in 3D TIs further indicate that axial anomaly is a universal phenomenon in generic 3D metals.

Over the last decade, numerous theoretical and experimental studies on topological states of quantum matter have revolutionized research in condensed matter physics. These materials possess a huge potential for tabletop experiments and advance technological applications such as topological quantum computing, spintronics and low-dissipation electronics$^{1,2}$. Topological insulators (TIs) are one such class of topological quantum matter that have bulk energy gap with conductive Dirac-cone-like topological surface states (TSSs) over the crystal boundary. The gapless metallic surface states of TIs are protected by time-reversal symmetry (TRS) and immune to scattering by non-magnetic impurities, thus opening new avenues for elastic scattering free transport applications. The binary Bi-based chalcogenides Bi$_2$Se$_3$ and Bi$_2$Te$_3$ have been regarded as reference 3D TIs with a relatively simple electronic structure consisting of single Dirac-cone TSS within the bulk energy gap at the centre of the Brillouin zone ($\Gamma$-point)$^{3,4}$. These materials have been extensively investigated previously for their efficient thermoelectric properties. The existence of robust and exotic TSS in Bi$_2$Te$_3$ has been previously demonstrated by several groups via low-temperature quantum transport measurements$^{5-7}$. As the electrical conduction in this narrow band-gap TI material is constantly plagued by residual bulk carriers, most of the experimental studies have been performed in low-dimensional geometries such as nanowires, nanoribbons, etc. where surface contribution is dominant.

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Magnetoresistance (MR) measurements provide very useful information about the type of conduction mechanism in the various materials. It is well known that conductivity corrections resulting from the quantum interference of time-reversed closed loops around an impurity or scattering point give rise to weak localization (WL) or weak antilocalization (WAL) effects, which can be directly observed through MR measurements. WAL or WL effect is more pronounced when phase coherence length exceeds the mean free path of the quasi-particle. These quantum-mechanical interference phenomena strongly depend on the temperature and are only observable at very low temperatures. In TIs, WAL effect is expected to manifest as a cusp-like feature in the MR curve at zero magnetic (B) field due to the presence of strong spin-momentum locking of the metallic TSS that leads to a π-Berry phase and suppresses backscattering. The WAL feature has been observed in many TI materials under out-of-plane perpendicular B-field. It was also shown in many studies that these conductivity corrections are highly influenced by the interaction of TSS and bulk carriers, thickness of the TI films, electron-electron (e-e) interaction and presence of disorder, where a crossover from WAL to WL can be observed. Parallel B-field MR provides an efficient way to investigate the bulk TI states, as it is very difficult to distinguish the bulk states properties from TSS under perpendicular B-field. It has been shown that magneto-transport measurements under in-plane B-field applied parallel to the sample plane can provide an efficient way to detect bulk conduction contribution and surface-to-bulk coupling. WL or WAL effect can also arise under parallel B-fields due to some finite thickness of the sample material, where Aharonov-Bohm (AB) phase can be acquired by the closed loop electron trajectory encircling certain amount of B-flux while undergoing inter-surface or surface-to-bulk scatterings.

Recent demonstration of axial or chiral anomaly in Weyl semimetals via negative MR (NMR) under parallel B-field has generated tremendous interest in studying the properties of NMR in different topological materials. NMR was observed in magnetic materials and Anderson localized 2D electron gas. The observation of NMR under parallel B-field in materials other than topological semimetals without any Weyl nodes has led to the belief that NMR is a generic property of metallic or semiconducting materials. Till date, several NMR observations have been reported in TIs under both perpendicular and parallel B-fields, for example, in ultrathin Bi<sub>2</sub>Se<sub>3</sub> films due to crossover between WL and WAL of bulk electrons, in ultrathin (Bi<sub>x</sub>Sb<sub>1−x</sub>)<sub>2</sub>Te<sub>3</sub> films due to opening of energy gap in TSS that modifies the Berry phase and leads to competing WL and WAL at low B-fields, in ultrathin (Bi<sub>x</sub>Sb<sub>1−x</sub>)<sub>2</sub>Te<sub>3</sub> films due to disorder-induced Anderson localization, in Sn-doped Bi<sub>2</sub>Te<sub>3</sub> polycrystalline films and Bi<sub>x</sub>(Te<sub>0.6</sub>Sb<sub>0.4</sub>)<sub>y</sub>, films due to WL effect of bulk states, in Bi<sub>2</sub>Se<sub>3</sub> nanoribbons due to Zeeman energy induced surface Dirac cone deformation and spin-dependent scattering of TSS, in Bi-rich Bi<sub>2</sub>SbTe<sub>3</sub> nanoflakes due to disorder induced enhancement of defect states density from Ar+ ion milling, in TiBi<sub>0.15</sub>Sb<sub>0.85</sub>Te<sub>3</sub> due to formation of charge puddles in disordered bulk, in epitaxial Bi<sub>2</sub>Se<sub>3</sub> thin films due to underlying scattering mechanisms and in Bi<sub>x</sub>Se<sub>1−x</sub> due to non-trivial bulk conduction and appearance of electron puddles from sulphur doping. Thus, there is a growing interest to understand the underlying mechanism for the origin of NMR in non-magnetic TIs.

In this study, we report the observation of NMR under in-plane B-field applied parallel to the current direction in focused-ion-beam (FIB) fabricated Bi<sub>2</sub>Te<sub>3</sub> nanowires. Temperature dependent interplay between NMR and positive MR (PMR) has been observed in all the nanodevices. The direction of the B-field is same for entire study. Large NMR of −22% at 8 T is observed in one of the devices at 0.3 K, which is significantly higher considering TI without magnetic doping. Various physical phenomena such as competition between dephasing and spin-orbit scattering time, Ga<sup>+</sup> ion milling induced disorder and contamination leading to strong localization, electron hopping transport, charge puddle formation and spin accumulated localized regions have been discussed for possible explanation of NMR. The first-principles calculations within a density-functional theory (DFT) framework show that Ga<sup>+</sup> induced disorder (substitutional) in the Bi<sub>2</sub>Te<sub>3</sub> crystal gives rise to local magnetic moments in the material. Qualitative analysis of the effect of orientation of B-field, excitation current and spin-polarization of the TSS along-with the bulk conductance interference can explain the origin of NMR and other MR characteristics observed in all the devices via spin-dependent scattering mechanism of surface and bulk electrons on local magnetic moments.

**Results and Discussion**

**Experimental analysis.** Parallel orientation of B-field to the plane of the sample (B<sub>||</sub>) has always been a source of some peculiar and rich physical phenomenon in TI materials, where the strong spin-momentum locking of the TSS generates a spin-polarized current under application of electric field. An in-plane B-field applied perpendicular to the current direction (B<sub>⊥</sub> || I) perfectly aligns parallelly with the spin polarization direction and when in-plane B-field is applied parallel to the current direction (B<sub>||</sub> || I), there occurs a perpendicular orientation between B-field and spin-polarization of TSS that results into unusual MR behaviour. The same is evident from Fig. 1 in our case with Bi<sub>2</sub>Te<sub>3</sub> nanowire devices under B<sub>||</sub> || I orientation. Figure 1a–c depict the percentage MR change (longitudinal MR) with applied parallel B-field for devices SH-1, 2 and 5 at different temperatures. The MR change (%) can be written as

\[
MR\ change\ (%) = \frac{R(B) - R(0T)}{R(0T)} \times 100\%
\]

where R(B) and R(0T) is the resistance at any B and 0 T, respectively. We observe a temperature dependent competition between the PMR and NMR in all the devices. NMR is mostly prevalent at ultralow temperatures (T < 2 K). With increasing temperature, a shifting trend from NMR to PMR is observed for all the devices. Although, sample SH5 (Fig. 1c) does not show complete PMR till 5 K, but still there starts a decreasing NMR slope since 1 K. This reflects the fact that the observed NMR phenomenon is strongly dependent on the temperature. Another significant observation in this direction is the decreasing MR change (%) with increasing temperature in all the devices.
For device SH2 (Fig. 1b), a high MR change of $-22\%$ (at 8 T) is observed at ultralow temperature of 0.3 K, which gradually decreases to around 1.5% at 8 K. This decay of NMR with increasing temperature suggests the presence of some temperature dependent quantum-mechanical property related to the orientation of spin-polarization of TSS and B-field.

It must be noted that, we did not observe any periodic MR oscillations (in Fig. 1) corresponding to the cross-sectional area of the Bi$_2$Te$_3$ nanowire arising from AB interference effect of TSS, which has been previously shown to be a hallmark of TSS existence under $B//I$\cite{5,6,31}. Rather, we have observed aperiodic MR fluctuations in the data, which is most likely the result of universal conductance fluctuations (UCF)\cite{32} or quantum interference of closed loop electronic trajectories with random cross-sectional areas. With increasing temperature, a PMR starts to appear at around 1.5 K for devices SH-1, 2. For device SH5 complete PMR is expected at a higher temperature than 5 K. PMR occurs in $B//I$ orientation due to the finite thickness of the sample, where AB phases are acquired by electron wave-functions enclosing some B-flux\cite{14,15}. The resulting quantum interference effect of self-intersecting closed paths modifies the conductivity of the sample. As we do not observe any flux quantization period corresponding to the cross-sectional area of the nanowire, therefore, we infer that high bulk conduction is present in our Bi$_2$Te$_3$ nanowire samples. The interference of bulk states with TSS can easily host such random electron trajectories leading to arbitrary AB phases and aperiodic MR oscillations. Previous reports on Bi$_2$Te$_3$ material have also demonstrated the presence of high bulk conductance contribution, where gate voltage or doping was used to suppress the bulk conductivity and realize TSS transport\cite{5,13}.

Figure 1d depicts the competition between PMR and NMR in Bi$_2$Te$_3$ nanowire devices. The MR at ultralow temperature of 0.05 K can be divided into three regimes, viz., regime-1 with small NMR, regime-2 with small PMR and regime-3 with large NMR extending till very high B-fields. The different regimes for devices SH-1 and 5 range from 0 to 1 T for regime-1, 1 to 3 T for regime-2 and 3 to 10 T (which is the highest B-field used in this study) for regime-3. The main panel of Fig. 1d shows that, strangely enough, the MR for devices SH-1 and 5 enter and exit any of the regimes at around same B-field value. Also, at different temperatures (till 0.3 K) for device SH5, we observe that MR enters and exits any regime at same B-field value. But, this is not the case with device SH2, where only two regimes (regime-1 and 2) can be seen till 10 T at $T=0.05$ K (inset in Fig. 1d). At 0.05 K, initially NMR is present till 2.7 T followed by PMR till 10 T. Although at 0.1 and 0.2 K, again three MR regimes were found within 10 T. For 0.1 K (inset in Fig. 1d), regimes-1, 2 and 3 extend from 0 to 1.16 T (NMR), 1.16 to 3.5 T (PMR) and 3.5 to 10 T (NMR). Similarly for 0.2 K (Fig. 1b), regimes-1, 2 and 3 extend from 0 to 0.8 T (NMR), 0.8 to 2.3 T
NR19,34. Whereas, under strong localization regime (Anderson localization, $\tau_{\text{SO}}$ fact that some additional physical mechanism is dominant in our samples that leads to the observed high with increasing B-field. Thus, the occurrence of NMR in all the devices under this orientation is indicative of the asymmetry in the spin-up and spin-down density of states (DOS), generating local magnetic moments in the parallel, which leads to decreased spin-orbit scattering and high $\tau_{\text{SO}}$ sequence of the fact that for $B_{\parallel I}$, B-field and spin-polarization direction of TSS (due to applied electric field) are parallel, which leads to decreased spin-orbit scattering and high $\tau_{\text{SO}}$. In our case, we find a crossover phenomenon and huge NMR for $B_{\parallel I}$ in Bi$_2$Te$_3$ nanowires. This is obviously much unexpected because in this orientation, B-field becomes perpendicular to the spin-polarization direction of TSS. As spin-flips leading to the alignment of B-field and spin-polarization direction are hindered by the strong in-plane perpendicular spin-momentum locking of TSS, therefore, $B_{\parallel I}$ orientation does not decrease the spin-orbit scattering and a PMR is expected with increasing B-field. Thus, the occurrence of NMR in all the devices under this orientation is indicative of the fact that some additional physical mechanism is dominant in our samples that leads to the observed high $\tau_{\text{SO}}$.

Previously, in ultrathin Bi$_2$Se$_3$ nanoribbons synthesized using chemical vapour deposition method, NMR under both transport in VRH regime and spin accumulated localized regions could lead to observed NMR under B-field. This intermediate regime is manifested as a crossover from WL to WAL or vice-versa. For regime-3, $\tau_{\text{SO}}$ $\gg$ $\tau_{\phi}$, which suggests very weak or negligible spin-flips leading to huge decrease in resistance. This can be observed as large NMR (WL effect) in the devices. For device SH5, regime-3 shows a large linearly decreasing MR with increasing B-field.

In another report, Banerjee et al. demonstrated the origin of NMR due to Ar ion milling process to fabricate the Bi$_2$Te$_3$ nanowires. It is well known that ion milling process induces slight disorder in the system. There can be some deformation and contamination in the material due to highly energetic Ga ions, which can create defect states. In our previous report on FIB-fabricated narrow Bi$_2$Se$_3$ nanowires, we had experimentally found the evidence of Efros-Shklovskii VRH mechanism, which is usually dominant in highly disordered systems. This suggests the possibility of strong localization effects in this case with Bi$_2$Te$_3$ also, where defect states from ion milling can bring the system transport in VRH regime and spin accumulated localized regions could lead to observed NMR under B-field. Previously, in Bi$_2$Se$_3$ nanoribbons synthesized using chemical vapour deposition method, NMR under both $B_{\parallel I}$ and $B_{\perp I}$ orientation was attributed to the Zeeman effect on TSS transport. It was proposed that due to the large Landé factor ($g$ $\approx$ 50) of Bi$_2$Se$_3$ surface electrons, Zeeman energy from $B_{\parallel I}$ will deform the Dirac cone leading to small spin-polarization of TSS. Also, the anti-site defect in Bi$_2$Se$_3$ due to Bi atom replacing one Se atom produces asymmetry in the spin-up and spin-down density of states (DOS), generating local magnetic moments in the
system. So, there occurs a spin-dependent scattering of surface electrons on local magnetic moments leading to NMR.

In our current study, it is possible that under $B_{||}I$ orientation, such spin-dependent scattering mechanism for NMR is present. As stated before, the interaction of Ga$^+$ ion with Bi$_2$Te$_3$ material, while fabricating Bi$_2$Te$_3$ nanowire from exfoliated Bi$_2$Te$_3$ nanoflake using FIB can introduce disorder in the system. Since, this fabrication technique is top-to-bottom approach (i.e. from nanoflake to nanowire) and milling is done from one of the sides of the nanoflake with other side remaining unaffected, therefore, we assume that most of the Ga$^+$ interaction is limited to only one side surface of Bi$_2$Te$_3$ nanowire. Bi$_2$Te$_3$ crystal structure consists of quintuple layers, i.e., five monatomic sheets of Te$_1$-Bi-Te$_2$-Bi-Te$_1$ stacked together with van der Waals (vdW) gap in between the quintuple layers (QLs) [40]. The Te$_1$-Te$_1$ bond is the weakest while the Bi-Te$_2$ bond is the strongest. Therefore, mechanical exfoliation usually results into cleaving the crystal into the vdW gap and breaking of Te$_1$-Te$_1$ bond. The two types of interaction or disorder in the crystal structure of Bi$_2$Te$_3$ by Ga are possible, viz., interstitial defect with Ga$^+$ ion being trapped inside the vdW gap and breaking of Te$_1$-Te$_1$ bond. The two types of interaction or disorder in the crystal structure of Bi$_2$Te$_3$ by Ga are possible, viz., interstitial defect with Ga$^+$ ion being trapped inside the vdW gap and breaking of Te$_1$-Te$_1$ bond. This may occur due to the Te vacancy caused by highly energetic Ga$^+$ ion, which can strike out Te atom from its site. This Ga$^+$ ion may acquire an electron and stabilize at the Te vacancy site. This can cause a line defect and dislocation in that QL. Since, the Bi-Te$_2$ bond is stronger than Bi-Te$_1$ bond [40], therefore, we focus on Ga occupying the Te$_2$ atomic site. Thus, we expect an asymmetric spin-resolved DOS near the Fermi energy leading to local magnetic moments that induces spin-dependent scattering of bulk and surface electrons.

In order to further investigate the origin of WL-like feature at zero B-field, we perform the Altshuler and Aronov (AA) fitting of the conductance correction ($\Delta G = G(B) - G(0T)$) versus B data. Equation 2 represents the AA formula [15,41] that describes the quantum correction to conductivity under $B_{||}I$ orientation.

$$\Delta G = G(B) - G(0T) \cong -\frac{\alpha e^2}{\pi \hbar} \ln \left(1 + \frac{\beta (eL_v/\hbar)^2}{B^2}\right)$$  

where $e =$ electronic charge, $\hbar =$ Planck’s constant, $\hbar = \hbar/2\pi$, $t =$ thickness of the nanowire and $L_v =$ electron dephasing length. The pre-factor $\alpha$ provides information about the strength of spin-orbit interaction (SOI) in the material with $\alpha = 0, 0.5$ and $-1$ for strong magnetic scattering, WAL with strong SOI and WL with weak SOI,
and local magnetic moment, there is higher probability for electron to move forward than being scattered backwards; and for anti-parallel alignment of both spin-up and spin-down electrons from both surface and bulk conduction channels in absence of exchange interaction energy. Also, there is reduced spin scattering of bulk electrons as their spins align with minority spin states are coloured in green and violet. We can see that the DOS of two spin states is equal, concentrating the existence of local magnetic moments at surface. Excitation current (I) is applied into the conduction region. The substitutional defect, where Ga replaces Te₂, shows small imbalance in the two spin-resolved DOS with Ga interstitial defect, where Ga is trapped inside the van der Waals gap (see Fig. 3f) is out-of-the-plane spin component develops and the Dirac cone becomes hexagonal warped. The spin-momentum locking feature of the surface state spin-texture leads to the absence of backscattering over the surface. The spin-resolved DOS with Ga interstitial defect, where Ga is trapped inside the van der Waals gap (see Fig. 3f) is shown in Fig. 3g. It is found that the Ga interfacial defect does not generate any imbalance between the majority and minority spin-states. However, if uniformly electron dope the system, thereby moving the Fermi level more into the conduction region. The substitutional defect, where Ga replaces Te₂, shows small imbalance in the two spin-states, indicating the existence of local magnetic moments. A first atomic analysis further reveals that Bi₂Te₃ QL with Ga defect possesses a local magnetic moment of 0.14 μₛ where a major contribution to magnetic moment comes from guest Ga atom. Such local magnetic moments due to substitutional defects have been reported earlier for Ga interstitial defect, we place Ga atom in the van der Waals gap and perform full structural relaxation.

In order to understand the effect of Ga defects, we first study the topological properties of pristine Bi₂Te₃. The conventional bulk hexagonal unit cell is shown in Fig. 3a. It consists of 15 atomic layers that are grouped into three QLs. The associated spin-resolved density of states (DOS) is shown in Fig. 3b. The DOS of the majority and minority spin states are coloured in green and violet. We can see that the DOS of two spin states is equal, consistent with its nonmagnetic ground state with TRS. A clear band gap can be seen between the occupied valence and unoccupied conduction states. The slab band structure of Bi₂Te₃ in Fig. 3c resolves a single topological Dirac cone surface state that connects bulk valence and conduction bands. The Dirac point overlaps in energy with bulk valence continuum and lies at an energy ~0.1 eV. The spin-texture and Dirac cone structure of the upper portion of the TSS are shown in Fig. 3d,e, respectively. The spin is clearly constrained perpendicular to the momentum over a substantial region of k-space around the Dirac point. As one moves away from the Dirac point a finite out-of-the-plane spin component develops and the Dirac cone becomes hexagonal warped. The spin-momentum locking feature of the surface state spin-texture leads to the absence of backscattering over the surface. The spin-resolved DOS with Ga interstitial defect, where Ga is trapped inside the van der Waals gap (see Fig. 3f) is shown in Fig. 3g. It is found that the Ga interfacial defect does not generate any imbalance between the majority and minority spin-states. However, if uniformly electron dope the system, thereby moving the Fermi level more into the conduction region. The substitutional defect, where Ga replaces Te₂, shows small imbalance in the two spin-states, indicating the existence of local magnetic moments. A first atomic analysis further reveals that Bi₂Te₃ QL with Ga defect possesses a local magnetic moment of 0.14 μₛ where a major contribution to magnetic moment comes from guest Ga atom. Such local magnetic moments due to substitutional defects have been reported earlier for Ga interstitial defect, we place Ga atom in the van der Waals gap and perform full structural relaxation.

Electronic structure analysis. To develop a better understanding of the experimental results, we have computed electronic structure of Bi₂Te₃ with Ga defects within DFT framework as implemented in the Vienna Ab initio Simulation Package (VASP). We use projector augmented wave method to treat interaction between ion cores and valence electrons and generalized gradient approximation to consider exchange-correlation effects. All the results presented here are obtained using the fully relaxed structural parameters. The plane wave-cut off energy of 310 eV is employed and a 12 × 12 × 8 Γ-centred k-mesh is used for bulk computations. We use a slab model with a vacuum of 12 Å to avoid interaction between periodically repeated slabs and 9 × 9 × 1 Γ-centred k mesh to obtain the surface states. In order to resolve the Dirac cone and spin structure of TSS, we carry out computations on a finer k-mesh around the surface Brillouin zone centre and conventional hexagonal supercell with sixty atomic layers. Ga substitutional defect is modelled by replacing one Te₂ atom from the ideal position in pristine Bi₂Te₃ structure, whereas, for Ga interstitial defect, we place Ga atom in the van der Waals gap and perform full structural relaxation.

Figure 4 shows the schematic of the electron transport and scattering mechanism in our FIB-fabricated Bi₂Te₃ nanowires under zero B-field (Fig. 4a) and B // || orientation (Fig. 4b). As confirmed by the DFT analysis (Fig. 3), Ga⁺ disorder due to milling process does produce some local magnetic moments in the material. Also, it is expected that Ga⁺ implantation and contamination will be at surface of the sample only, therefore, Fig. 4 depicts some Ga impurity atom with localized process of magnetic moments at surface. Excitation current (I) is applied along the nanowire length. When surface or bulk electron encounters a localized region, then the interaction between electron spin (σₑ) and local magnetic moment (μₛ) can be explained by the exchange energy βσₑ ⋅ μₛ, where β is the exchange interaction strength. Fig. 4a shows the scattering mechanism for B = 0 T, where the local magnetic moments are randomly oriented. Depending on the angle between σₑ and μₛ, the scattering of electron occurs. For parallel σₑ and μₛ, there is higher probability for electron to move forward than being scattered backwards; and for anti-parallel σₑ and μₛ, backscattering probability is high. Thus, we have a spin-dependent scattering of both spin-up and spin-down electrons from both surface and bulk conduction channels in absence of exchange interaction energy. Also, there is reduced spin scattering of bulk electrons as their spins align with B and local magnetic moments. Therefore, the significantly reduced spin-dependent scattering of both surface and bulk electrons from localized magnetic moments under B || leads to high τₑ which decreases the sample resistance and causes NMR. The crossover from NMR to complete PMR with increasing temperature can be attributed to the diminishing density of local magnetic moments due to thermal energy.
In our previous report on FIB-fabricated Bi₂Se₃ nanowire, we found signatures of periodic AB oscillations from TSS with dominant $h/e$ flux quantization period⁴⁶. There was no observation of NMR in any of the Bi₂Se₃ nanowires for $T \geq 2$ K. However, we did find evidences of modified surface electron path due to FIB-induced disorder and Ga contamination indicating the robustness of TSS to non-magnetic disorder. Recently, few experimental reports have validated the existence of robust TSS in FIB-fabricated TI nanostructures and shown the promising nature of FIB technique towards fabrication of desired TI-based nanostructure geometries⁴⁶–⁴⁹. In this study, high bulk conductivity of Bi₂Te₃ and ultralow temperatures (down to 20 mK) may have led to the observation of NMR due to enhanced localization and spin-scattering related effects on quantum transport. For regime-1, the sharp NMR cusp near 0 T can be attributed to the WL effect of bulk Bi₂Te₃ channels. Previous theoretical⁵⁰ and experimental⁴⁶ reports have demonstrated that WL is expected for bulk TI bands, and whenever the bulk WL channels outnumber the TSS WL channels, NMR due to WL effect is observable. The strength of spin-orbit coupling is very strong in the bulk of 3D TI Bi₂Te₃ and ideally the bulk states should also demonstrate WL effect at low fields similar to the TSS. However, unlike the gapless TSS, the gapped bulk states have relatively large bulk bandgap, which may result into WL effect. As under parallel B-field orientation, a large number of bulk channels contribute to the quantum transport, therefore the overall WL effect in regime-1 can be interpreted as the collective result of multiple bulk transport channels. The competition between the two types of scattering channels “bulk WL channels” and “bulk WL channels” decides the overall magneto-transport behaviour of the system. Also, it is known that sample fabrication introduces some disorder and defects in the system. Thus, it becomes

Figure 3. Electronic properties of Bi₂Te₃ with Ga defects. (a) Conventional hexagonal unit cell with 15 atomic layers that are grouped in three QLs. Each QL has Te₁-Bi-Te₂ atomic stacking with strong bonds between the layers whereas two QLs are held together by weak Van der Waals forces. (b) Total spin-resolved bulk DOS of $2 \times 2 \times 1$ supercell of pristine Bi₂Te₃ with a clear band gap between the occupied valence and unoccupied conduction states. (c) Calculated slab band structure of Bi₂Te₃. Shaded background grey region highlights projected bulk bands and blue thick lines identify slab bands. The TSS are clearly resolved within the bulk energy gap. (d) Helical spin-texture and (e) Dirac cone electronic structure of the top cone of TSS. In-plane spin-texture is shown with black arrows in (d). (f) Bi₂Te₃ QLs with Ga interstitial and substitutional defects. Ga atoms slide into the van der Waals gap in interstitial defects whereas these replace Te₂ atoms in substitutional defects. Total spin-resolved $2 \times 2 \times 1$ bulk DOS for (g) interstitial defect and (h) substitutional defect.
highly likely that the bulk WL channels will outnumber the bulk WAL channels and lead to WL cusp or NMR. In regime-2 at low B-fields, we have high spin-orbit scattering rates (low $\tau_{SO}$) due to the scattering of both spin-up and spin-down electrons from surface and bulk on some randomly oriented local magnetic moments that do not align completely parallel with the B-field direction due to low B-field strength. This scattering leads to slight increase in resistance and thus, PMR in regime-2. However, under the influence of strong B-field in regime-3, these local magnetic moments align parallel to the direction of B-field, which leads to significant decrease in the spin-dependent scattering (high $\tau_{SO}$) of surface and bulk electrons on local magnetic moments and causes resistance to decrease, i.e., NMR in regime-3.

In a recent turnover of events, it was theoretically and experimentally shown that the appearance of charge imbalance in generic 3D metals due to parallel orientation of electric and magnetic field, similar to the chiral anomaly effect in Weyl semimetals, makes axial anomaly a universal phenomenon not specific to Weyl or Dirac semimetals. It was also predicted that axial anomaly does not guarantee NMR. NMR phenomenon under $B_{||} \parallel I$ is not just dependent on the electronic band structure of a material, but also on the type of scattering mechanism in the sample. In case of ionic impurity scattering, strong NMR can be observed and in presence of both neutral and ionic impurities, a crossover from NMR to PMR can be observed under $B_{||} \parallel I$ for any 3D or quasi-2D metal in the quantum limit. Occurrence of such a longitudinal NMR has been proposed as a hallmark of bulk transport in topological phases of matter. This reflects the fact that longitudinal NMR observed in 3D TIs and other non-topological materials is a condition- and sample-specific complicated phenomenon that needs many more experimental and theoretically efforts to fully explain the underlying mechanism.

**Conclusion**

The observation of large NMR in TI Bi$_2$Te$_3$ nanowires at ultralow temperatures ($T < 2$ K) has been reported in this work. Strong temperature dependence of NMR suggests some quantum mechanical phenomenon as the origin. MR switch to PMR with increasing temperature was observed. Similar type of MR characteristics have been observed for all the nanodevices indicating some common physical mechanism intrinsic to the material. WL and WAL-like features arising from NMR and PMR have been discussed via competing dephasing and spin-orbit scattering time scales. Different mechanisms reported to cause NMR in the past such as disorder-induced localization of electronic states, VRH transport, formation of charge puddles and ion-milling enhanced defect density in the material were discussed. Spin polarized DFT calculations confirm the presence of spin-dependent scattering of surface and bulk electrons on local magnetic moments created by Ga$^+$ disorder as the reason for observed temperature dependent NMR. A very speculative comparison with universal axial anomaly phenomenon in generic 3D or quasi-2D metal in the quantum limit under $B_{||} \parallel I$ orientation is done. We believe that validation of
universal axial anomaly in 3D TIs will require further experiments towards estimation of the quantum limit and MR characteristics at ultrahigh B-fields (~50 T) giving access to lowest Landau level.

**Experimental Methods**

Focused-ion-beam (FIB) milling technique was used to fabricate the Bi$_2$Te$_3$ nanowires from micro-mechanically exfoliated thin flakes deposited on SO$_2$/Si substrates. The substrates were pre-cleaned via chemical (acetone, iso-propanol, methanol and de-ionized water), ultrasonication and 10 min oxygen plasma treatment. Thick Au/Ti (~80/5 nm) contacts were deposited on the substrates using DC sputtering to serve as electrical contacts. Bi$_2$Te$_3$ bulk crystals from Alfa Aesar company were used to exfoliate thin flakes using standard Scotch-tape method. The very thin nanoflakes were localized under optical microscope (Olympus MX51) and field emission scanning electron microscopy (FESEM by Zeiss-Auriga). The thickness of the localized thin nanoflakes was determined via atomic force microscopy (AFM) and cross-sectional FESEM techniques. FIB milling using Ga$^+$ ions was performed to mill nanoflake into nanowire. After that, FIB-based gas injection system (GIS) was used to deposit Pt electrodes connecting pre-sputtered gold contacts and nanowire. Four-probe geometry was designed for electrical measurements. The width, thickness and channel length (distance between two voltage measuring electrodes) of the nanowires used in this study are: ~114 nm, ~50 nm and ~547 nm for SH1; ~302 nm, ~45 nm and ~866 nm for SH2; and ~282 nm, ~56 nm and ~652 nm for SH5, respectively. Insets in Fig. 1a–c show the FESEM images of the devices SH1, 2 and 5, respectively. See Supplementary file for the elemental characterization of Bi$_2$Te$_3$ sample. The low temperature electric transport measurements were done in a dilution refrigerator (Triton 200, Oxford Instruments) with a base temperature of 10 mK and with a 14 T uniaxial magnet. The measurement leads were incorporated with RF filters at room temperature (cut off frequency of 100 MHz) to avoid EMI due to high frequency RF radiation reaching the sample stage. A bias current of 10 nA (17 Hz) derived from a lock-in-amplifier (Signal Recovery 7265) through a series resistor of 1 MΩ is used for the entire magneto-resistance measurements.

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Author Contributions
S.H. planned and supervised the study. S.H. and B.B. fabricated the nanodevices. R.P.A. performed low temperature DR measurements. B.S. and S.A. performed DFT calculations, analyzed and wrote the DFT results. C.S. and H.L. assisted with the literature survey and microscopy sample preparation. A.G. and T.D.S. provided FIB materials, laboratory tools and DR facility. B.B. and S.H. carried out the experimental data analysis, image graphics, manuscript writing and preparation. All authors read and commented on the manuscript.

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