Crossover from weak-antilocalization transport to quantum magnetoresistance of Dirac states in quenched Fe$_{0.01}$Bi$_2$Te$_3$ single crystals with large magnetoresistance and high Hall mobility

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Keywords: topological insulator, Hall mobility, quantum magnetoresistance, weak-antilocalization transport

Abstract
Magnetotransport properties with a large positive magnetoresistance (MR) and a high carrier mobility for applications have been achieved and probed for quenched Fe$_{0.01}$Bi$_2$Te$_3$ single crystals. Large positive MR of $\sim$470% with a Hall mobility of $\sim$44 000 cm$^2$ V$^{-1}$ s$^{-1}$ at 5 K and 6 T has been observed on a quenched Fe$_{0.01}$Bi$_2$Te$_3$ sample, in which the electrical parameters can be tuned by the quenching temperature $T_q$. The MR behaviors for the quenched samples show a crossover from a weak antilocalization-dominant MR to a linear and non-saturating MR at temperatures of $T^* \approx 58 - 100$ K, where the large MR at low temperatures possibly originates from the mechanism of topologically protected backscattering. On the contrary, the MR behaviors for the strain-released sample do not show such a distinct crossover, where only linear-like and non-saturating MR behaviors can be observed. Different electrical transports between the quenched and strain-released samples indicate that the band structure, as well as the surface Dirac electrons in Fe$_{0.01}$Bi$_2$Te$_3$, can be modified by the lattice strain. Furthermore, it is found that the low-temperature magnetococonductivity can be well described by the weak-antilocalization transport formula, while the high-field linear-like MR at $T > T^*$ can be explained in terms of Abrikosov’s quantum transport of Dirac-cone states in quenched Fe$_{0.01}$Bi$_2$Te$_3$ single crystals.

1. Introduction
Magnetically doped topological insulators (MTIs), emerging as a new light on the subject of dilute magnetic semiconductors, have attracted much attention in recent years due to their potential applications in spintronic devices [1, 2]. To date, intense efforts have been made regarding intentional magnetic doping of topological semiconductors. Ferromagnetism of MTIs has been reported in Fe and Mn-doped Bi$_2$Te$_3$ [3–5], Co and Fe-doped Bi$_2$Se$_3$ [6–8], Cr-doped Sb$_2$Te$_3$ [9], and V-doped (Bi,Sb)$_2$Te$_3$ [10]. In particular, the stability, electronic, and magnetic properties of the MTIs Bi$_2$Se$_3$, Bi$_2$Te$_3$, and Sb$_2$Te$_3$ have been predicted and provided important guidance for magnetism incorporation in MTIs experimentally [11]. The ferromagnetism in the topological insulator (TI) is expected to break the time-reversal symmetry, in which this complicated interplay between the topological order and ferromagnetism inspired many proposals to realize exotic quantum phenomena [2, 12]. The quantum spin/anomalous Hall effect and Dirac fermion-mediated magnetic coupling physics have achieved a spotlight in topological transports of MTIs. Surprisingly, for spintronic applications only a few attempts [13–15] have been made at the magnetoresistance (MR) and carrier-mobility effects in MTIs. It is known that a TI having photon-like electrons in it, is characterized by the linear dispersion relation between the energy and momentum. This property can improve the performance of semiconductor devices resulting from high sensitivity to the external electrical field of the topological surface, i.e. high carrier mobility, $\mu$. In practical applications, high carrier mobility allows a TI-based device to have a fast running speed and high cut-off frequency [2]. Such properties will make MTIs particularly interesting for spintronic applications because high-
mobility devices are expected to achieve longer spin diffusion lengths due to the low scattering rate, as seen in organic semiconductors and graphene-based devices [16, 17]. This is especially important when scaling down the supply voltage and thus, reducing the power density in advanced technologies. An extremely large MR (XMR) and an ultrahigh mobility have been reported only in the so-called topological Dirac and Weyl semimetals, such as Cd3As2 ($\mu = 9 \times 10^6$ cm$^2$ V$^{-1}$ s$^{-1}$ at 5 K, MR = 1.5 × 10% at 1.5 K and 14.5 T) and NbP ($\mu = 5 \times 10^6$ cm$^2$ V$^{-1}$ s$^{-1}$ at 1.85 K, MR = 8.5 × 10% at 1.85 K and 9 T), respectively [18, 19]. Among the MTIs, high-mobility Sm-doped Bi$_2$Te$_3$, in which the Hall mobility can reach more than $10^4$ cm$^2$ V$^{-1}$ s$^{-1}$ accompanied with ferromagnetism up to about 52 K, was reported [13]. Curiously enough, so far only a high-mobility TI, Bi$_2$Se$_3$, with a high magnetoresistance has been reported, in which the carrier Hall mobility was also up to $10^4$ cm$^2$ V$^{-1}$ s$^{-1}$ and a large positive linear MR approaching 400% without any sign of saturation was observed at 1.4 K and 14 T [14]. Recently, it was shown that doping of non-magnetic Cu in Bi$_2$Te$_3$ TIs induced ferromagnetism at room temperature and also enhanced the magnetoresistance, where a rather large MR of $\sim 1000$% with a low $\mu$ of $\sim 10^2$ cm$^2$ V$^{-1}$ s$^{-1}$ for Bi$_2$Cu$_{0.15}$Te$_{2.85}$ at 2 K and 10 T was reported [15]. More recently, in Zn doped Bi$_2$Te$_3$ single crystals, a large positive MR of $\sim 400$% at 2 K and 7 T with a mobility value of $\sim 7200$ cm$^2$ V$^{-1}$ s$^{-1}$ was reported [20]. So far, these TIs show a common magnetotransport characteristic in which a weak antilocalization (WAL) effect can be observed at low temperatures accompanied by a non-saturating linear-like MR at higher temperatures [14, 15, 20–23]. This particular linear-like MR has been explained by Abrikosov’s ‘quantum linear MR’ mechanism [24] and a classic model proposed by Parish and Littlewood [25]. The relationship between the MR of MTIs and carrier mobility, however, has not been completely revealed, even though a considerable number of theoretical and experimental studies have been conducted on MR behavior in topological materials over the past few years [2, 26].

On the other hand, it has been pointed out that the TI properties in the Bi$_2$Te$_3$ alloy easily decay within a time scale of a few months due to surface contaminations, leading to this material not being suitable for stable application use [5]. In contrast to the undoped Bi$_2$Te$_3$, it has been reported that Fe-doped Bi$_2$Te$_3$ alloys have a TI behavior similar to the clean surface Dirac electrons and the TI properties have an extremely long lifetime, which is very important for the applications [3]. Here, we report a large positive MR of nearly 470% at 5 K and 6 T, and a corresponding high mobility of up to $4.4 \times 10^4$ cm$^2$ V$^{-1}$ s$^{-1}$ obtained in our quenched Fe-doped Bi$_2$Te$_3$ single crystals with an atomic Fe dopant ratio of $\sim 1$%. At room temperature, samples also show a positive MR of $\sim 10$%, which is comparable to that observed in colossal-MR manganites [27]. Samples were synthesized via a conventional self-flux method with different temperatures of quenching in cold water in order to control the strain in the lattice structure. It was found that large values for the MR and Hall mobility for the samples can be achieved and tuned by quenching temperature $T_q$. Furthermore, the origins of transport and relationship between the MR and carrier mobility in our Fe-doped Bi$_2$Te$_3$ single crystals are being debated. In particular, although a large number of studies have been made on the Bi$_2$Te$_3$, single crystals, little is known about the special magnetotransport properties of magnetically doped samples with quenching.

2. Experiments

Single crystals of Fe$_{0.01}$Bi$_2$Te$_3$ were grown by the self-flux method using starting materials of Fe, Bi, and Te powders. High-purity elements were mixed in at a molar ratio of Fe:Bi:Te = 0.01:2:3 and sealed in an evacuated quartz tube. The tube was heated up to 900 °C for 48 h for melting stoichiometric mixtures of high-purity elements. Crystal growth took place via slow cooling at a rate of $-3$ °C h$^{-1}$ from 900 °C to the quenching temperature $T_q$, annealing at $T_q$ for 48 h, and then quenching in cold water to vary the lattice strain in the Fe-intercalated Bi$_2$Te$_3$ crystals, where the values of $T_q$ were 560 °C, 480 °C, and 400 °C, respectively. In addition, a strain-released sample was grown in slow cooling at a rate of $-10$ °C h$^{-1}$ from 900 °C to room temperature without the quenching process. Thus, the studied Fe$_{0.01}$Bi$_2$Te$_3$ single crystals can be denoted as S560, S480, S400, and S$_{Ch}$ for growth with $T_q$ of 560 °C, 480 °C, 400 °C and a strain-released sample, respectively. Powder x-ray diffractometer (D2 PHASER with Cu $K_{\alpha}$ radiation) was employed to characterize the crystal structure of samples. The compositions have been determined by means of Energy dispersive x-ray spectroscopy done at different sites for each sample and show a homogeneous Fe distribution with a ratio of $\sim 1$% atomic Fe dopant. For in-plane transport measurements, the cleaved shiny crystals were cut into dimensions of $\sim 3.0 \times 1.0 \times 0.1$ mm$^3$. The crystal $c$ axis determined by the x-ray diffraction was perpendicular to the plane of the crystal slabs. Five leads were soldered with indium, and a Hall-measurement geometry was constructed to allow simultaneous measurements of both longitudinal ($\rho_{xx}$) and transverse (Hall) resistivities ($\rho_{xy}$) using the standard dc four-probe technique. Hall voltages were taken in opposing fields parallel to the $c$-axis up to 6 T and at a dc current density of $\sim 30$ A cm$^{-2}$. The magnetization was measured in a superconducting quantum interference device system (MPMS from Quantum Design).
3. Results and discussion

Figure 1 (a) shows the x-ray θ–2θ diffraction spectra for samples S560, S480, S400, and Ssr in which only the (00n) (n = 6, 15, 18, and 21) diffraction peaks were observed, indicating that the [001] direction is perpendicular to the plane of the crystals. The inset in figure 1 (a) shows the x-ray θ–2θ diffraction spectra in the region near the (0015) peak for corresponding samples. The peaks are broad and have a shoulder at a higher 2θ angle due to the Cu–Kα1 and Cu–Kα2 radiations. As can be seen, the (0015) peak of S560 positions is at a lower angle due to a slight increase in the length of the c axis. As seen, the peak position shifts to a smaller 2θ angle for samples with a higher Tq. The lattice constants of the c axis can be determined precisely to be: 30.477, 30.471, 30.464, and 30.418 Å for samples S560, S480, S400, and Ssr, respectively. The lattice constant of Ssr is very close to that of 30.43 Å for the undoped Bi2Te3 single crystal reported by Singh et al. [20]. Figure 1 (b) shows the quenching temperature Tq dependence of the c-axis lattice constant. As seen, the c-axis lattice constant increases with the increase in quenching temperature Tq. The inset of figure 1 (b) shows the quenching temperature Tq dependence of the c-axis strain ε, which is calculated from the x-ray diffraction results. Here, strain ε is determined by ε = |c − csr|/csr, where c is the c-axis value for the Ssr sample. As shown, the ε value increases with the increase in Tq, corresponding to the observation of an increased strain ε value for samples with a higher quenching temperature. The increased strain can be attributed to the strain induced by the lattices that are crystallized from the early stage of quenching. Furthermore, according to the larger c-axis lattice constants observed in the quenched samples compared with that of Ssr, we can infer that the doped Fe atoms in the quenched samples are mostly located at the intercalated van der Waals gap positions, since they are not at the substitutional position with Bi. On the contrary, if the Fe impurities in Bi2Te3 are substituted into the Bi site in a 2+ oxidation site, therefore one can see that the c-axis lattice constant should be smaller because of the smaller ionic radius of Fe2+. A detailed description of the Fe-ion intercalation in Bi2Te3 probed by the x-ray diffraction, Hall measurement, and spectra of synchrotron x-ray photoemission spectroscopy will be reported elsewhere.

Magnetization results (see details in the supplementary figure S1 is available online at stacks.iop.org/NJP/22/013012/mmedia) show a diamagnetic characteristic without ferromagnetic hysteresis and saturation at 2.5 K observed in the magnetization versus field (M–B) curves. Hence the hysteresis loss of energy does not occur while these materials are used for spin-electronic applications. The non-ferromagnetic property has also been confirmed with the absence of hysteresis loops in Hall effect measurements as shown in the supplementary
The diamagnetic characteristic without ferromagnetic hysteresis is likely to originate from a large diamagnetic response in Bi$_2$Te$_3$, and a very weak ferromagnetism of Fe dopants as briefly discussed in the supplementary material. Basic electrical transports of zero-resistance $\rho$, and the Hall coefficient $R_H$ for the quenched and strain-released Fe$_{0.01}$Bi$_2$Te$_3$ samples are also provided in the supplementary figure S2. Data display a metallic conduction for samples with a progressively increasing resistivity as the temperature increases. The $R_H$ values studied at whole temperatures are negative and signify that electron-type carriers dominate the electrical transport in the quenched samples, while positive $R_H$ values at whole temperatures for the strain-released sample can be observed. The observed electron-dominant carriers are in accordance with previous inference that most of the Fe impurities in quenched Fe$_{0.01}$Bi$_2$Te$_3$ do not substitute into the Bi$^{3+}$ oxidation site in which numerous hole-type carriers will be contributed.

Figure 2(a) shows a typical main result of MR behavior for sample S480 with $B$ fields applied perpendicular to the crystalline $ab$ plane. Here, the MR of the samples is defined as MR$\% = [R(B) - R(0)]/R(0) \times 100\%$, where $R(B)$ is the resistance at the applied magnetic field $B$, and $R(0)$ is the measured resistance at $B = 0$. As shown in figure 2(a), the MR increases with the applied fields but decreases with the increase in temperature, and a clear non-saturating MR can be seen for the entire range of temperature and field of measurement. A sharp resistance dip is clearly observed at low temperatures, and as the temperature increases, the MR dip at a low $B$ is broadened indicating the reduction of the surface state. Furthermore, the MR becomes linear for the intermediate temperature range and at higher temperatures it shows a quadratic-like behavior in the low-field region. As mentioned previously, a sharp resistance dip at low temperatures is an indication of the presence of a WAL effect and as we increase the temperature, the MR dip broadens at the low field because the phase coherence length decreases at higher temperatures [22]. Looking closely at the field-dependent MR, one can see that it is completely symmetric for the entire range of measured temperatures with respect to the reversal of the magnetic field direction. The MR behavior at higher fields of $>1.5$ T can be approximately described by MR$\% \propto B^{\alpha}$. Figure 2(b) shows ln(MR) as a function of $\ln(B)$ for the corresponding data in figure 2(a) with some selected temperatures and illustrates the dependence of MR$\% \propto B^{\alpha}$. The inset of figure 2(b) shows the temperature dependence of $\alpha$ values, which are in the range of 0.5–1.4. It is obvious from the $\alpha(T)$ graph that $\alpha < 1$; this corresponds to the presence of an MR dip at temperatures below 75 K, while $\alpha \geq 1$ at temperatures above 100 K. This result indicates a crossover from a WAL-dominant MR to a clear linear and non-saturating MR at a temperature of $T^{*} \approx 100$ K. In contrast to the MR behavior of S480, figures 3(a) and (b) show the MR
results and $\ln(\text{MR})$ as a function of $\ln(B)$ for sample Ssr, respectively. The inset of figure 3(b) shows the temperature dependence of $\alpha$ values with $\alpha \approx 1.0$ at a temperature of $T^* \approx 5$ K, indicating that there is no distinct crossover from a WAL-dominant MR to a clear linear MR.

Table 1 illustrates the $c$-axis lattice constants and basic electrical transport parameters, including room-temperature resistivity $\rho_{xx}(300 \text{ K})$ and $\rho_{xx}(5 \text{ K})$, MR(6 T) values at 5 and 300 K, carrier concentration $n(5 \text{ K})$, carrier Hall mobility $\mu(5 \text{ K})$, and temperature $T^*$ for all samples studied. Different electrical transports between the quenched and strain-released Fe$_{0.01}$Bi$_2$Te$_3$ samples are illustrated.

| Samples | $c$ (Å) | $\rho_{xx}(300 \text{ K})$ ($10^{-4} \Omega \text{ cm}$) | $\rho_{xx}(5 \text{ K})$ ($10^{-4} \Omega \text{ cm}$) | MR(5 K) (%) | MR(300 K) (%) | $n(5 \text{ K})$ ($10^{18} \text{ cm}^{-3}$) | $\mu(5 \text{ K})$ ($\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) | $T^*$ (K) |
|---------|--------|-----------------------------|-----------------------------|-------------|-------------|-------------------------------|-----------------------------|---------|
| S560    | 30.477 | 11.37                       | 0.386                       | 438         | 9.7         | $-6.30$                       | 25 661                      | 58      |
| S480    | 30.471 | 8.195                       | 0.262                       | 459         | 9.5         | $-6.06$                       | 39 262                      | 100     |
| S400    | 30.464 | 10.30                       | 0.294                       | 473         | 8.9         | $-4.82$                       | 44 081                      | 64      |
| Ssr     | 30.418 | 31.44                       | 2.595                       | 153         | 5.9         | $+7.00$                       | 3433                        | 5       |

As shown, a crossover from a WAL-dominant MR to a linear and non-saturating MR at a temperatures of $T^* \approx 58$ and 64 K can also be clearly observed on samples S560 and S400, respectively. In addition, the observed maximum MR for the S400 sample reaches 473% at 5 K and 6 T, which is much higher than the MR values that have been reported in the MTIs [3, 13, 14, 20–23].
carrier mobility is evaluated using the relation $\mu = 1/(\rho_{xx}|e|)$, where $e$ is the charge of the electron and $\rho_{xx}$ is the electrical resistivity at a zero magnetic field [28]. It can be seen that the nature of the electronic transport in the lightly Fe-doped Bi$_2$Te$_3$ single crystals indeed changes with the quench temperature and annealing, as recently reported on the annealed Bi$_2$SeTe$_2$ single crystals [29], in which lower mobility values for annealed Bi$_2$SeTe$_2$ samples were reported. Here, a smaller MR value of $\sim 150\%$ with a lower mobility value of $\sim 3400$ cm$^2$ V$^{-1}$ s$^{-1}$ for the strain-released Fe$_{0.01}$Bi$_2$Te$_3$ sample with a hole-dominant conductivity can also be observed (see details in figure 4, and the supplementary figures S2 and S5). For the quenched Fe$_{0.01}$Bi$_2$Te$_3$ samples, one can see that both the MR (5 K) and $\mu$ (5 K) values decrease with an increase in $T_q$. The distinctly different electrical transports between the quenched and strain-released samples also indicate that the band structure, as well as the surface Dirac electrons in Fe$_{0.01}$Bi$_2$Te$_3$, can be modified by the lattice strain in crystal structure.

Figures 4(a)–(c) show the temperature dependences of the MR, carrier concentration $n$, and Hall mobility $\mu$, which were determined with $B = 6$ T, for the quenched and strain-released samples, respectively. As seen, the values of MR and $\mu$ decrease with the increase in temperature, while the absolute values of carrier concentration $n$ increase with the increase in temperature for all samples. The increases in $|n|$ values as the temperature increases can be attributed to the increased bulk contribution and comes in the reported values of $\sim 10^{19}$ cm$^{-3}$ at 300 K [15, 20]. The inset of figure 4(a) displays a typical resistivity variation in the field of 6 T and zero field for the S560 sample. The inset of figure 4(b) shows a $\ln(|n|)$–$\ln(T)$ plot for the corresponding data of the quenched samples in (b). The inset of (c) demonstrates a $\ln(\mu)$–$\ln(T)$ plot for the corresponding data of the quenched samples in (c). The dashed lines illustrate the power-law dependences as described in the text.

Hence, it is clear that as we increase the temperature, mobility decreases. This is as expected because with the
increase in temperature, the carrier–carrier scattering and thus, the thermal vibration or contribution of carrier-phonon scattering increases. Consequently, the transport mean free path of the carriers, l_{\text{ex}} as well as the mobility, $\mu$, decrease because $\mu = e l_{\text{ex}} / (\hbar k_F)$ where $k_F$ is the Fermi wave number and $\hbar$ is the reduced Planck constant. A similar trend has been observed in other topological materials [15, 20].

Returning to the real subject of the field-dependent MR observed on Si408, it is known that there have been many attempts made to explain the mechanisms of the MR behavior, in particular, the linear and non-saturating MR in topological materials, as mentioned previously. In addition to the Abrikosov’s ‘quantum linear MR’ mechanism [24] and the classic Parish and Littlewood’s model (PL model) [25], Zhang et al have demonstrated that the strong linear-like MR at a high field for Bi\textsubscript{2}Te\textsubscript{3} films can be well understood as the WAL phenomena described by the Hikami-Larkin-Nagaoka (HLN) theory [23]. After looking deeper into their fittings to the magneto-conductivity (MC) data, however, deviation in low fields has been observed, accompanying the characteristic of a low-field quadratic-like MR observed at higher temperatures which seemingly does not match up well with their HLN equations. So far little attention has been given to the relationship between the large MR and carrier mobility in some MTIs [13, 14]. Recently, Sun et al have proposed that LaBi single crystals also exhibit a large MR, which can be ascribed to the nearly compensated electron and hole with a rather high mobility [30]. Their analysis has suggested that the XMR, as well as the field-induced resistivity upturn and plateau observed in LaBi, can be explained well by a two-band model with a compensation situation. According to this electron-hole compensation mechanism, however, quadratic-like behavior in MR is presented, being incompatible with the linear-like MR observed in topological materials. Moreover, all the studied samples reveal an ordinary Hall effect (as seen in the supplementary figures S2 and S5), and thus one can exclude the electron-hole compensation mechanism for Fe\textsubscript{0.01}Bi\textsubscript{2}Te\textsubscript{3}. The PL model has been proposed to solve the mystery of the linear MR found in disordered systems such as silver chalcogenides [31]. This model has claimed that the high-field MR in inhomogeneous conductors is independent of the carrier density and can be given by $B^\text{s} \approx \mu B$ with a crossover field which can be estimated by $B_c \approx \mu^{-1} [25]$. Taking into account the PL model, it has been argued that the behavior of observed MR in Bi\textsubscript{2}Se\textsubscript{3} nanoplates or Zn-doped Bi\textsubscript{2}Te\textsubscript{3} can be explained with the PL model, according to the estimated $B$, of ~1 T, which is consistent with the observed MR curves [14, 20]. To examine this model closely, in figure 5(a) we plot the $\ln(\mu)$ against the mobility $\ln(\mu)$ for the quenched samples. It can be seen that the mobility dependence of MR in the high-mobility region is roughly obeying $\mu \propto p$ with $p = 0.76 \pm 0.01$, obviously deviating from $p = 1$ predicted in the PL model. Furthermore, taking $B = 6$ T and $\mu$ of $2.5 - 4.4 \times 10^6 \text{cm}^2\text{V}^{-1}\text{s}^{-1}$ for our quenched samples into the PL formula of $\mu \approx \mu B$, the estimated MR is in the range of 1500%–2640%, which is much greater than the obtained MR in the range of ~440% – 470%. In figure 5(b) we show the $\ln(\mu)$ versus the carrier concentration $\ln(\mu)$ for samples in which a strong dependence of $\mu \propto |\mu|^{-4}$ with $q = 4.54 \pm 0.22$ can be roughly derived in the high-MR region. Considering the universal relationship of $\mu \propto l_{\text{ex}} \propto |\mu|^{-2/3}$ and $\mu \propto p$ predicted in the PL model, these results indicate that a better explanation for the observed MR behavior may not be close to the PL model. In view of this disagreement, we then consider the ‘quantum linear MR’ mechanism for understanding MR behavior. Within the framework of quantum mechanism by Abrikosov, however, it has been proposed that the estimated crossover field of ~10 T, arising from a high carrier concentration of ~$10^{19}$ cm$^{-3}$, is much greater than those of ~1 T [14, 20]. To address this, Abrikosov pointed out that with the assumption of material inhomogeneity, regions with higher electron concentrations are imbedded into regions with much smaller electron concentration. Hence, we infer that the assumption of material inhomogeneity, where regions with higher electron concentrations are imbedded into regions with much smaller electron concentration, an extremal quantum situation can take place in the small-concentration regions [24]. This assumption offers an interpretation of the experimental results that the dependence of the MR deviates from linearity only at $H < 10$ Oe for silver chalcogenides. Thus, before we come to the adequacy of the quantum MR mechanism, the possibility of carrier inhomogeneity in doped Bi\textsubscript{2}Te\textsubscript{3} must be clarified. With scanning tunneling microscopy analysis for the Bi\textsubscript{2–x}Mn\textsubscript{x}Te\textsubscript{3} single crystals, Hor et al have shown that the Mn substitutes on the Bi sites forming compounds of the type Bi\textsubscript{2–x}Mn\textsubscript{x}Te\textsubscript{3} and the Mn substitutions are randomly distributed [32]. Hence, we infer that the Fe substitutes in Bi\textsubscript{2}Te\textsubscript{3} can also be randomly distributed at the intercalated van der Waals gap positions, leading to carrier inhomogeneity in samples, even though there is no Fe elemental inhomogeneity observed in the analysis by energy-dispersive x-ray spectroscopy, which may be limited by its sensitivity resolution. Therefore, it seems reasonable to suppose the fact that the high-field linear-like MR originates from the Abrikosov’s quantum MR. Similar transport phenomena for the Dirac-cone states in Ba(FeAs)$_2$ and FeSe single crystals have been interpreted also by applying Abrikosov’s theory [33, 34]. This subject will be discussed further later on.

Having observed the crossover from a WAL-dominant MR to a linear and non-saturating MR at temperatures of $T^* \approx 58–100$ K and having noticed the possibility of Abrikosov’s quantum MR in our quenched Fe\textsubscript{0.01}Bi\textsubscript{2}Te\textsubscript{3} single crystals, one can then inspect the origin of the large MR values observed at low temperatures. It is known that except for the electron-hole compensation mechanism, the magnetic field lifting of topologically protected backscattering in topological semimetals could also lead to XMR [18]. In these systems, the backscattering is strongly suppressed at a zero field, resulting in a transport lifetime $\tau_0$ that is much longer.
than the quantum lifetime $\tau_Q$. To check this possible mechanism of XMR in Fe$_{0.01}$Bi$_2$Te$_3$, firstly we estimate the mean free path of carriers via the universal formula of $l_f = \frac{1}{2\pi v_F^2} \left( \frac{1}{\tau} \right)^{1/3} \frac{1}{|n|^{1/2}}$, yielding mean free paths of $\sim 1600$ nm for sample S480 at 2.5 K. Therefore, the transport lifetime $\tau_{tr}$ can be calculated to be $\sim 4.3 \times 10^{-12}$ s via $\tau_{tr} = l_f / v_F$, where $v_F$ is the Fermi velocity taken with $v_F = 3.7 \times 10^5$ m s$^{-1}$ [21]. Otherwise, the quantum lifetime $\tau_Q$ can be deduced from the measurement of Shubnikov-de Haas (ShD) oscillations by using $\tau_Q = \frac{\hbar}{2\pi k_B T_D}$, where $T_D$ is the Dingle temperature [18].

According to the reported ShD oscillations for a Bi$_2$Te$_3$ crystal [35], we estimate the $T_D$ to be $\sim 3.5$ K, and have a $\tau_Q$ value of $\sim 3.5 \times 10^{-13}$ s for our Fe$_{0.01}$Bi$_2$Te$_3$. Indeed, the transport lifetime $\tau_{tr}$ is much longer than the quantum lifetime $\tau_Q$, but the obtained ratio $\tau_{tr}/\tau_Q$ of $\sim 12$ for Fe$_{0.01}$Bi$_2$Te$_3$ is around a three order of magnitude smaller than that of $\sim 10^4$ for XMR-semimetal Cd$_2$As$_2$ [18]. Thus, topologically protected backscattering is a possible mechanism for large MR values of our Fe$_{0.01}$Bi$_2$Te$_3$ at low temperatures. The small $\tau_{tr}/\tau_Q$ ratio for Fe$_{0.01}$Bi$_2$Te$_3$ may be due to some magnetic scatterings that opens the backscattering channel via the spin–flip process and degrades the state’s coherence.

Now that the magneto-transport property of quenched Fe$_{0.01}$Bi$_2$Te$_3$ indicates a crossover from a WAL-dominant MR to a linear and non-saturating MR at a temperature of $T^*$, the field-dependent MR will be analyzed within the framework of a WAL electrical transported and quantum linear MR at $T < T^*$ and $T > T^*$, respectively. Figure 6(a) shows a typical field-dependent transverse magnetoconductivity (MC) change ratio for S480 at low temperatures, where the MC change ratio $\Delta MC$ is defined as $\Delta MC = |\sigma(B) - \sigma(0)|/\sigma(0)$. It is known that the transverse MC can be expressed by $\sigma(B) = \sigma_{WAL} + \sigma_n$, where $\sigma_{WAL}$ is the surface conductivity from WAL corrections associated with intranode scattering, and $\sigma_n$ is from conventional Fermi surface contributions [36]. The WAL formula is given by $\sigma_{WAL} = a \sqrt{B} + \sigma_0$ and $\sigma_n = (\rho_0 + A B^2)^{-1}$, where $a$, $\sigma_0$, $\rho_0$ and $A$ are determined from the line of best fit. As seen, the transverse MC indeed can be well described by the WAL transport formula. Figure 6(b) shows the temperature dependences of obtained $a$ and $A$ values. As seen, parameter $a$ is negative due to a positive MR and is weakly dependent upon temperature at temperatures below 10 K, in accordance with the prediction of theory [37]. At higher temperatures, the decrease in $|a|$ values with an increase in temperature indicates a gradual absence of the WAL effect on the field-dependent transverse MC. In addition, within the presented theory, parameter $A$ originates from the classical orbital MR and is proportional to the transport scattering time $\tau_n$ [38]. Since $\tau_n(T) \propto 1/\rho_{xx}(T)$, a plot of $1/|A|$ versus $\rho_{xx}$ should fall on a straight line. In the inset of figure 6(b) we show the linear $\rho_{xx}$ dependence of $1/A$ for samples S400, S480 and S560 and illustrate a clear consistency between the data and theoretical prediction.

Figure 5. (a) A plot of $\ln(\text{MR})$ against the mobility $\ln(\mu)$ for the quenched samples. The dashed lines denote the dependence of $\text{MR} \propto \mu^p$ with $p = 0.76 \pm 0.01$. (b) A plot of $\ln(\text{MR})$ versus the carrier concentration $\ln(|n|)$ for the quenched samples. The dashed lines illustrate the power-law fitting of $\text{MR} \propto |n|^{-q}$ with $q = 4.54 \pm 0.22$. 

![Figure 5](image-url)
Turning to the subject of high-field Abrikosov’s quantum MR for S480 at $T > T^*$, a crossover of MR values from a semi-classical weak field $B^2$ dependence to a nearly linear $B$ dependence can be observed when the magnetic field is beyond critical field $B^*$. The critical field $B^*$ can be determined by the plot of differential MR versus the field, $dMR/db$, as typically shown in figure 7(a). As seen, $dMR/db$ is linearly proportional to $B$ with a large positive slope in low fields but reaches a nearly constant value when the field is higher than $B^*$, which is determined by an intersection of two linear fitting lines, as shown by the guide lines in figure 7(a). One can see that the critical field $B^*$ for all the quenched samples shifts to a higher field with the increase in temperature, as shown in figure 7(b). The temperature dependence of the critical field suggests the existence of an electronic band with a linear dispersion in Fe$_{0.01}$Bi$_2$Te$_3$ [33]. Actually, according to another model of the quantum linear MR in layered semimetals proposed by Abrikosov [39], an applied magnetic field will induce the Landau level (LL) splitting; in the quantum limit at a specific temperature and a field, LL spacing will then become larger than both the Fermi energy $E_F$ and the thermal fluctuations $k_BT$. As a result, only the lowest LL is occupied for the small Fermi pockets and a quantum linear MR appears. Furthermore, it has been deduced that the splitting between the lowest and the first LL, $\Delta_1$, with $\Delta_1 = E_F + k_BT$ at critical field $B^*$, could satisfy the regime of the quantum limit. Therefore, the $B$-linear MR originates from the Dirac cone states, and the observed $B^*(T)$ corresponds to the limit of $B^*(T) = (1/2e\hbar v_F^2)(E_F + k_BT)^2$ [24]. The critical field $B^*(T)$ can be examined via the plot of $\sqrt{B^2}$ versus $T$, as shown in the inset of figure 7(b). As shown, the temperature dependence of critical field $B^*$ can be well fitted with the $\sqrt{B^2} - T$ plotting. The fitting results yield Fermi level $E_F \approx 12, 13, \text{ and } 10 \text{ meV}$; and Fermi velocity $v_F \approx 5.4 \times 10^5, 6.1 \times 10^5, \text{ and } 5.2 \times 10^5 \text{ m s}^{-1} \text{ for samples S400, S480, and S560, respectively.}$

The yielded $v_F$ values are close to that of $3.7 \times 10^5 \text{ m s}^{-1}$, as previously mentioned. On the other hand, we estimated the Fermi level to be around 0.014 eV above the bottom of the bulk conduction band (BCB) based on the electron concentration of $n(100 \text{ K}) \approx 8 \times 10^{18} \text{ cm}^{-3}$ and the formula $E_F = \frac{\hbar^2}{2m_e} (3\pi^2 n)^{2/3}$, where $m_e$ is the electron mass. In addition, from the band structure calculations [11], the Fe-doped Bi$_2$Te$_3$ has been suggested to be semimetal with a narrow gap of 2.4 meV, so the whole Fermi energy is $\approx 0.016 \text{ eV}$ with respect to the Dirac point. Thus the estimated $E_F$ of 16 meV is also near those of 10–13 meV obtained from the $B^*(T)$ fitting, which satisfies the regime of the quantum limit. Thus, according to the $E_F$ values obtained from the critical field $B^*$ and referring to the band structure that was determined by angle-resolved photoemission spectroscopy (ARPES) measurements [40], the upper inset of figure 7 shows the sketch of the surface state dispersion where the solid lines indicate the obtained Fermi levels of samples S400, S480, and S560, and the dashed lines indicate the suggested band gap of 2.4 meV between BCB and bulk valence band [11]. In addition, the inference that the observed electrical transport is dominated by the surface Dirac electrons can also be confirmed by the MR measurements on samples with different thicknesses. In the supplementary figure S6 we show the MR behaviors at 5 K for S480 single crystals (from the same batch) with different thicknesses for comparison, where the
thickness $d = 20, 100, \text{ and } 460 \, \mu m$, respectively. As seen, larger MR values can be observed on the thinner samples, in which the contribution of bulk conductivity is reduced, further confirming that the MR behavior is indeed dominated by the surface Dirac-state electrons. These presented results strongly support the concept that linear MR behavior can be explained in terms of the quantum transport of Dirac-cone states in Fe$_{0.01}$Bi$_2$Te$_3$. This work also provides important experimental results for further studies on the doped topological materials, such as the theoretical band-structure calculation, ARPES experiments, as well as their magnetotransport properties, which are popular topics in condensed matter physics.

4. Conclusion

In conclusion, a large positive MR with a high carrier mobility has been observed on our quenched Fe$_{0.01}$Bi$_2$Te$_3$ single crystals. Stable values of MR and Hall mobility for the samples can be achieved and tuned by quenching temperature $T_{q}$, making this material suitable for applications. In addition, distinctly different electrical transports between the quenched and strain-released samples have been reported, indicating that the band structure, as well as the surface Dirac electrons in Fe$_{0.01}$Bi$_2$Te$_3$, can be modified by the lattice strain. Furthermore, this study explored the origins of magnetotransport properties and the relationship between the MR and carrier mobility for the samples can be achieved and tuned by quenching temperature $T_{q}$, making this material suitable for applications. In addition, distinctly different electrical transports between the quenched and strain-released samples have been reported, indicating that the band structure, as well as the surface Dirac electrons in Fe$_{0.01}$Bi$_2$Te$_3$, can be modified by the lattice strain. According to the fact that the transport lifetime $\tau_{opt}$ is much longer than that of the quantum lifetime $\tau_{Q}$, it is concluded that topologically protected backscattering is a possible mechanism for the observed large MR values at low temperatures, where the transverse MC can also be well described by the WAL transport formula. Finally, a high-field linear-like MR at $T > T^*$ has been examined within the framework of Abrikosov’s quantum MR theory. It has been found that critical field $B^*(T)$ could satisfy the regime of quantum limit and can be examined via the plotting of $\sqrt{B^*}$ versus $T$, and thus a schematic band structure with a surface Dirac-cone state for samples is illustrated with Fermi levels in BCB. Our results strongly support the concept that linear MR behavior can be explained in terms of Abrikosov’s quantum transport of Dirac-cone states in quenched Fe$_{0.01}$Bi$_2$Te$_3$ single crystals.
Acknowledgments

The authors thank the National Science Council of the Republic of China for financial support under grant number MOST 107-2112-M-002-018.

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