Signature of the topological surface state in the thermoelectric properties of Bi$_2$Te$_3$

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We present ab initio electronic structure calculations based on density functional theory for the thermoelectric properties of Bi$_2$Te$_3$ films. Conductivity and thermopower are computed in the diffusive limit of transport based on the Boltzmann equation. Bulk and surface contribution to the transport coefficients are separated by a special projection technique. As a result we show clear signatures of the topological surface state in the thermoelectric properties.

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Recent studies in condensed-matter physics showed that Bi$_2$Te$_3$, which is one of the most studied and efficient thermoelectric materials¹,², belongs to the group of Z2 topological insulators³–⁵. Clearly the link between an efficient thermoelectric material and the topological character is the spin-orbit induced inverted band gap. While the small size of the band gap favours room-temperature thermoelectrics⁶, the inversion itself often occurs by heavy atoms, leading to low lattice thermal conductivity enhancing the figure of merit. In addition, the existence of topological surface states opens the opportunity to increase the performance of thermoelectric devices⁷–⁹.

While many experiments and calculations were performed investigating the robustness and the spin texture of the gapless surface state in Bi$_2$Te$_3$⁵,¹⁰,¹¹, the precise identification of the surface states contribution to the various transport coefficients is still an open question¹²,¹³.

We present ab initio calculations of the thermoelectric transport properties of a Bi$_2$Te$_3$ film. The transport properties of the Bi$_2$Te$_3$ film are calculated in the diffusive limit of transport by means of the semiclassical Boltzmann equation in relaxation time approximation (RTA)¹⁴–²⁰. Within this approximation we assume that the attached metallic leads basically preserve the surface band structure.

The electronic structure of the Bi$_2$Te$_3$ surface was obtained by first principles density functional theory calculations (DFT), as implemented in the fully relativistic screened Korringa-Kohn-Rostoker Green function method (KKR)²¹. Exchange and correlation effects were accurately accounted for by the local density approximation (LDA) parametrized by Vosco, Wilk, and Nusair²². The atomic structure was simulated by a slab configuration of 20 atomic layers Bi$_2$Te$_3$, i.e. four quintuple layers (QL), separated by a vacuum spacer of sufficient thickness to separate the films. The experimental in-plane lattice parameter $a_{BiTe} = 4.384\text{Å}$ and relaxed atomic positions²³ were used. The calculated electronic bandstructure of the Bi$_2$Te$_3$ surface (black dots) is shown together with the projected bulk band structure (gray shaded areas) along the hexagonal high symmetry lines in Fig. 1(a). The findings are in good agreement with previous calculations²⁴–²⁶. The Dirac point of the Bi$_2$Te$_3$ gapless surface state is located deep inside the bulk valence bands, at about 168 meV below the bulk valence band maximum (VBM), clearly reinforced by the distinct indirect bulk band gap. As is known from theory²⁷ and experiment²⁸,²⁹ the hybridization of the surface states localized on both sides of the slab leads to an artificial band gap opening of the Dirac state in the order of a few meV. We observed a closure of the Dirac point band gap within an accuracy of 1 meV for 6 QL, albeit not showing any influence on the states character or the transport properties of the surface states.

With increasing Fermi level starting at the Dirac point the Fermi surface is circular, going to be hexagonal at $\approx 150$ meV (cf. Figs. 1(c),(d)) and getting snowflakelike above 270 meV (Fig. 1(b)). The origin of warping is the hybridization of the surface state with the bulk states in the $\Gamma\text{M}$ direction above 252 meV giving rise to a flat energy band, while in $\Gamma\text{K}$ direction the surface state stays isolated from the bulk states up to 0.8 eV. The Fermi velocities in the high-symmetry directions differ remarkably, by $v_{\text{F1}} / v_{\text{F2}} \approx 4$, over a large energy range $E_F - E_D \approx 0.25 - 0.5$ eV.

The DFT results serve as input to obtain the thermoelectric transport properties, using the layer-resolved transport distribution function (TDF) $\Sigma_{\parallel,\perp}(\mu) = \mathcal{L}_{\parallel,\perp}(\mu, 0)$³⁰,³¹. The generalized conductance moments $\mathcal{L}_{\parallel,\perp}(\mu, T)$ are defined as

$$\mathcal{L}_{\parallel}(\mu, T) = \frac{1}{2\pi^2} \sum_{\nu} \int d^3k \left| \psi_{k,\nu}^\parallel \right|^2 P_{\parallel,\nu} (E_k - \mu) \left( -\frac{\partial f_{\nu}(E_k, T)}{\partial E_k} \right)_{E_k = E_{\nu}}.$$  

Here the relaxation time for Bi$_2$Te$_3$ was fitted to experimental data and chosen to be constant in its absolute value $\tau = 11$ fs with respect to wave vector $k$ and energy

$$\int dr |\psi_k(r)|^2 = \sum_i P_{\parallel,\nu}^i = 1.$$  

v_{\text{F1}} / v_{\text{F2}} \approx 4$, over a large energy range $E_F - E_D \approx 0.25 - 0.5$ eV.
FIG. 1. (color online) (a) Band structure of the 30 layer Bi$_2$Te$_3$ slab (black dots) and surface projected bulk band structure (gray shaded areas). As an inset the surface Dirac state is highlighted. The Fermi surface at (b) 316 meV, (c) 270 meV and (d) 205 meV above the Dirac energy $E_D$ is shown. Superimposed onto the Fermi surfaces is the probability density (e)-(g) of the surface states. Red color indicates a pure surface state mostly localized in the outermost quintuple layers, as shown in (g). Blue color refers to bulk-like contributions to the surface states along the $\bar{\Gamma}-\bar{M}$ high symmetry line, as presented in (e) and (f).

on the scale of $k_B T$. No distinction of surface and bulk scattering was assumed to allow for a clear discussion of the electronic structure on the electronic transport. The influence of electron-phonon coupling was theoretically and experimentally found to be very weak and discussed more in detail in Appendix A. Straightforward, the temperature- and doping-dependent in-plane electrical conductivity $\sigma_\parallel$ and thermopower $S_\parallel$ read as

$$\sigma_\parallel = 2e^2 \mathcal{L}_\parallel^{(0)}(\mu, T) \quad \text{and} \quad S_\parallel = \frac{1}{e T} \mathcal{L}_\parallel^{(1)}(\mu, T)$$

for given chemical potential $\mu$ at temperature $T$ and carrier concentration $n$. All transport calculations presented below are performed with adaptive k-point mesh’s larger than 500 points on a piece of the 2D Fermi surface which lies in the irreducible part of the Brillouin zone and at least 150 000 (56 million k-points) k-points in the entire 3D BZ for the bulk TDF at low (high) charge carrier concentrations. Detailed descriptions were given in earlier publications by Ref. 33 and 34. By means of the layer-resolved probability amplitude $P_k(r)$ the thermoelectric transport properties can be decomposed into contributions of typical eigenstates. Within here, the distinction of surface states, characterized by a strong spatial localization in the outermost QL together with an exponential decay into the bulk and vacuum, and bulk states is required. This is done by probing a test eigenstate $\psi_{k,SS}(r)$ with the prototype surface eigenstate $\psi_{k,SS}(r)$ via $\xi_k = \int dr \psi_k^{*}(r) \psi_{k,SS}(r)$. If $\xi_k$ is larger than a given threshold close to one, the state $k$ is considered a surface state. An example for the latter is given in Fig. 1(g), by showing the layer-resolved probability amplitude. Most of the surface states probability amplitude is located at the outermost QL. Furthermore, the information of the states character is shown on the Fermi surfaces Figs. 1(b)-(d). It is seen that all states of the surface band crossing the band gap possess surface state character with the corresponding spatial distribution (Fig. 1(d)) up to an energy of about 220 meV above the Dirac point. From here, slight deviations of the state’s prototype surface state character occur (cf. Fig. 1(f)), as states in the $\bar{\Gamma}-\bar{M}$ direction show clear bulk like character with a high probability amplitude in the center of the layer, e.g. shown in Fig. 1(e). Consequently, $\xi_k \to 0$ and these states do not behave as typical surface states, although originating from the Dirac band. As indicated earlier the surface states band is unaffected by hybridization effects in the $\bar{\Gamma}\bar{K}$ direction up to $E_F - E_D \approx 0.8$ eV. As a result the Fermi surface show emerging bulk or surface character, most convincingly depicted in Fig. 1(b). As will be discussed hereinafter, this fact leads to a strong influence on the electronic transport, exceptionally stating an almost constant electrical surface conductivity.
over a broad doping regime.

Basis of all transport properties discussed below is the TDF \( \Sigma_{\parallel}(\mu) \), which can be understood as electrical conductivity at vanishing temperature. Due to hybridization, the TDF of the surface states contains contributions from surface and bulk states, which can be clearly separated using the projection technique by probability amplitudes as introduced above. We will distinguish between contributions from the pure surface state (SS) (cf. Fig. 1(g)), located at the surface, and bulk contributions to the surface states. The bulk TDF (gray shaded areas), as well as the surface (red solid line) contribution of the TDF are shown in Fig. 2. The TDF of the surface contribution rises almost linearly with energy. Having in mind, that for a two-dimensional system the TDF scales as \( \Sigma_{\parallel}(\mu) \propto d_F \times v_\parallel \), whereas \( d_F \) is the length of the Fermi circle at chemical potential \( \mu \), the linearity of the TDF in energy close to the Dirac point is obvious. Here, \( v_\parallel \) is constant with energy, while \( d_F \propto E \). Small deviations from the latter arise about \( E_F - E_D \approx 0.1 \text{ eV} \) and can be related to the hexagonal warping of the Fermi surface. At about 250 meV the increase of the TDF saturates and \( v_{SS}^{\parallel} \) remains roughly constant over a wide range of energy. As pointed out earlier, the pure surface states are not only spatially confined within approximately the outermost QL, but are also restricted to selected \( k \)-directions because of the hybridization with the bulk states. In the ultimate limit of \( k \)-selection only one Bloch function in \( \bar{\Gamma}\bar{K} \) direction with a constant Fermi velocity \( v_{\bar{\Gamma}\bar{K}} \) approximately realized for energies up to 0.8 eV above the Dirac point would be available for each surface state. As a consequence, the TDF of the surface state reads

\[
\Sigma_{\text{TD}}(\mu) = \frac{1}{\pi} \int d\mathbf{k} \left( v_{\bar{\Gamma}\bar{K}} \right)^2 \delta(\mu - v_{\bar{\Gamma}\bar{K}} k) = \frac{L v_{\bar{\Gamma}\bar{K}}^2}{\pi}.
\]

Obviously, the transition from the two-dimensional character of the surface states into a one-dimensional one changes the energy dependence of the TDF from linear into constant (cf. Fig. 2). With the TDF being directly related to \( L_{\parallel}^{(0)}(\mu, T) \) the electrical conductivity of the surface state is expected to be energy independent for electron doping as well. We note, the fact of the Dirac point being buried deep inside the bulk valence bands causes a surface contribution to the TDF only for energies larger than \( E_D \). In the following, we will discuss the doping- and temperature-dependent electrical conductivity and thermopower, as shown in Fig. 3. As done before, we will distinguish between contributions from bulk states (gray dashed lines), surface states (red solid lines) and the total contribution (black dash-dotted line), defined as \( \sigma_{\text{tot}} = \sigma_{\text{bulk}} + \sigma_{\text{SS}} \) and \( S_{\text{tot}} = (\sigma_{\text{bulk}} S_{\text{bulk}} + \sigma_{\text{SS}} S_{\text{SS}})/\sigma_{\text{tot}} \). Three typical charge carrier concentrations are chosen to reflect the overall behaviour of the transport properties.
Due to the mere fact that a three-dimensional topological insulator offers robust metal-like surface states in the insulating bulk band gap, an enhanced electrical conductivity of the whole system is expected for very small charge carrier concentrations, i.e. the chemical potential being situated in the bulk band gap. The temperature dependence of the electrical conductivity for such a scenario, at an electron doping of \( n = 1 \times 10^{18} \text{ cm}^{-3} \), is shown in Fig. 3(b). The surface contribution \( \sigma_{SS} \) of the electrical conductivity is almost temperature independent at approximately \( 105 \text{ (Ωcm)}^{-1} \) for the entire temperature range. This behaviour is a consequence of the earlier discussed energy-independence of the TDF for electron doping. For low temperatures \( \sigma_{SS} \) is up to 4 times larger than the bulk value of \( 28 \text{ (Ωcm)}^{-1} \) and the surface conductivity clearly dominates. For elevating temperatures bipolar bulk conduction leads to the well known exponential increase in \( \sigma_{\text{bulk}} \) for narrow band gap semi-conductors and \( \sigma_{\text{bulk}} > \sigma_{SS} \) holds for \( T > 300 \text{ K} \). Due to the independence of \( \sigma_{SS} \) on temperature the surface contribution to the total electrical conductivity is almost hidden and causes only a notable offset at low temperatures. However, such a behaviour was experimentally seen for thin \( \text{Bi}_2\text{Te}_3 \) films.\(^{37,38} \) A possibility to experimentally clarify whether surface states contribute to the total transport or not could be performed by measuring the total thermopower \( S_{\text{tot}} \) of the system, which decomposed in its parts is shown in Fig. 3(e). For the bulk contribution of \( S_{\text{tot}} \) the typical behaviour for a slightly doped narrow band gap bulk semiconductor is obtained. With increasing temperature the absolute value of \( \sigma_{\text{bulk}} \) rises linearly and the chemical potential shifts from the bulk conduction band into the bulk band gap. At a temperature of about 155 K large bulk values of the thermopower of \(-320 \mu\text{V/K}\) are obtained. At higher temperatures \( \sigma_{\text{bulk}} \) saturates at the expected small values because of bipolar intrinsic transport. For a bulk semiconductor in the intrinsic limit holds \( S_{\text{max}} \approx \frac{e \mu}{2 \hbar} \), the surface contribution \( S_{SS} \) shows the expected metal-like behaviour with absolute values well below \( \pm 10 \mu\text{V/K} \). This leads in sum to a clearly diminished total thermopower. More precisely, assuming that \( \sigma_{\text{bulk}} \gg S_{SS} \), it is \( S_{\text{tot}} \approx S_{\text{bulk}}/(\eta+1) \) for \( \eta = \sigma_{SS}/\sigma_{\text{bulk}} \). The maximal absolute value of the total thermopower (black dashed-dotted line in Fig. 3(e)) is found to be reduced to a fifth of the bulk value being \(-62 \mu\text{V/K} \) at 170 K, which corroborates the above-noted estimation. A clear transport contribution of the surface state will lead to a heavily decreased absolute value of the total thermopower.

To complete the picture two additional doping regimes will be discussed. Usually bulk \( \text{Bi}_2\text{Te}_3 \) is intrinsically electron-doped due to anti-site defects. In Fig. 3(a),(d) the electron doping amounts \( n = 2 \times 10^{19} \text{ cm}^{-3} \) and \( \mu \) lies in or close to the bulk conduction band. Here \( \sigma_{\text{tot}} \) is mainly defined by the bulk conductivity and reaches 685 (Ωcm)\(^{-1} \) at room temperature. The surface contribution is about 12-15% for all temperatures, being almost constant with temperature, again reflecting the weak energy-dependence of the TDF. With the surface thermopower expectantly behaving metal-like, but \( \sigma_{\text{bulk}} \gg \sigma_{SS} \), the surface states impact on \( S_{\text{tot}} \) is only moderate reducing \( S_{\text{tot}} \) just up to 15% of the bulk value.

Recent model calculations\(^{8,9} \) for \( \text{Bi}_2\text{Te}_3 \) proposed a dramatically enhanced thermoelectric powerfactor, i.e. \( S\mu \), at low temperatures and a location of the chemical potential near the Dirac point. To enter this regime, high hole doping rates are necessary. Here, we fixed the hole charge carrier concentration to \( p = 4 \times 10^{20} \text{ cm}^{-3} \) to discuss a possible enhancement of the thermoelectric powerfactor of \( \text{Bi}_2\text{Te}_3 \) in the presence of gapless metal-like surface states. Indeed, as is shown in Fig. 3(f), \( S_{SS} \) possesses large semiconductor-like absolute values, even showing a divergence for \( T \to 0 \), with \( \mu(T = 0) \) coinciding with the Dirac energy \( E_D \). This behaviour originates in the asymmetric slope of the TDF mocking a bulk band edge and yielding \( S_{SS} \sim -1/(\mu-E_D) \). Nevertheless the total thermopower and the bulk contribution to the thermopower are identical, both showing small positive values and a linear temperature dependence expected from a highly doped hole semiconductor. The reason is the heavily suppressed contribution of the surface states due to the large difference between \( \sigma_{SS} \) and \( \sigma_{\text{bulk}} \) as shown in Fig. 3(c). With the chemical potential deep in the bulk valence bands near the Dirac point, \( \sigma_{\text{bulk}} \) dominates the total electrical transport by about a factor 300 and with this the contribution of \( S_{SS} \) is negligible. If the Dirac point would be situated in the bulk band gap, i.e. available in \( \text{Bi}_2\text{Se}_3 \) and \( \text{Sb}_2\text{Te}_3 \), the electronic thermoelectric transport is most probably enhanced with respect to bulk behaviour. In \( \text{Bi}_2\text{Te}_3 \) such an enhancement is suppressed by the energetic position of the Dirac point, buried deep inside the bulk valence bands.

We furthermore note, that the thermodynamical limit \( S_{SS}(T \to 0) \to 0 \) is reached as soon as the temperature dependent chemical potential at zero temperature is not identical to the Dirac energy, i.e. \( \mu(T = 0) \neq E_D \). This is emphasized in Fig. 3(f) (blue thin dotted line) for a slightly smaller p-doping of \( p = 3 \times 10^{20} \text{ cm}^{-3} \). Here, \( \mu(T = 0) = E_D + 15 \text{ meV} \) and the thermopower of the surface state vanishes at zero temperature. The total thermopower \( S_{\text{tot}} \) of the thin film has always to vanish at zero temperature, regardless of the temperature dependence of the surface states’ contribution (c.f. Figs. 3(d)-(f)).

In conclusion, we presented \( \text{ab initio} \) calculations of the thermoelectric properties of \( \text{Bi}_2\text{Te}_3 \) films. The contribution of bulk and surface states to conductivity and thermopower are separated by a special projection technique. The contribution of the topological surface state is particularly pronounced in the low doping regime if the chemical potential lies in the bulk band gap.

The conductivity of the semi-conductor \( \text{Bi}_2\text{Te}_3 \) is enhanced by a constant contribution because of the surface state and reaches values of a metallic system. The thermopower of bulk semi-conductors shows a pronounced maximum as a function of temperature. The maximum
value is determined by the size of the band gap. With the existence of the topological surface state this maximum value is drastically reduced towards metallic behaviour. A reduction of the total thermopower has been found in various experiments on thin film thermoelectric topological insulators, i.e. Bi$_2$Te$_3$, Sb$_2$Te$_3$ and Bi$_{2−x}$Sb$_x$Te$_3$, with, up to now, no clear explanation$^{41−43}$.

Consequently, the measured thermopower can be used to prove whether a surface state exists and contributes to the transport properties. To clearly distinguish between a topological surface state and a trivial surface state we suggest measurements of the thermopower at a single crystal. The contribution of the topological surface state is expected to be independent from the single crystal orientation with respect to the current direction since the topological SS occurs on all surfaces$^{44}$, while a trivial SS is restricted to selected surfaces. Following our discussion, a reduction to metallic behaviour of the thermopower and electrical conductivity is expected for all orientations of the single crystal.

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Appendix A: Electron-phonon scattering

Electron-phonon interactions are up to now not explicitly accounted for in our ab initio calculations. The latter would most probably lead a priori to a 1/T behaviour of only the electron-phonon contribution to the bulk total relaxation time. Moreover we used the following ansatz for first estimations$^{45}$.

Applying Matthiessen’s rule the total electronic relaxation time, neglecting electron-electron and electron-magnon processes, reads as

$$\frac{1}{\tau} = \frac{1}{\tau_{el-imp}} + \frac{1}{\tau_{el-ph}}.$$  \hspace{1cm} (A1)

Within our manuscript the total relaxation time $\tau$ was fitted to experimental transport measurements. In particular the thermopower in dependence of the electrical conductivity $S(\sigma)$ was analysed as first suggested by Ref. 46. The total relaxation time was found to be $\tau = 11$ fs for n and p-doped bulk materials, which is in good agreement to other theoretically $\tau = 6−22$ fs$^{47}$ and experimentally determined $\tau = 36$ fs relaxation times$^{48}$. More details can be found in a previous publication$^{49}$.

Knowing the Éliashberg function $\alpha^2 F(\omega)$ allows to calculate the quasi-elastic electron-phonon scattering rate by$^{50}$

$$(\tau_{el-ph})^{-1} = 2\pi \int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} \times \{f^0(\epsilon_F + \hbar \omega) - f^0(\epsilon_F - \hbar \omega) + 2n^0(\omega) + 1\} \epsilon_F = 0 = 4\pi \int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\sinh(\frac{\hbar \omega}{k_B T})}. \hspace{1cm} (A2)$$

with the coupling constant defined as

$$\lambda = 2 \int_0^\infty \frac{\alpha^2 F(\omega)}{\omega} d\omega. \hspace{1cm} (A3)$$

Here, $n^0$ and $f^0$ are the Bose-Einstein and Fermi-Dirac distribution, respectively. Once all phonon modes can contribute to the electron-phonon scattering, i.e. $k_B T \geq \hbar \omega_{\text{max}}$ (for bulk Bi$_2$Te$_3$, i.e. $\omega_{\text{max}} \approx 17 \text{ meV}$), one readily obtains the relation $\tau_{el-ph} = (\frac{\hbar}{2\pi k_B T}) \frac{1}{\lambda}$ from eq. A2$^{51}$. Hence, in the high-temperature limit the scattering rate becomes linear in temperature, with a slope determined only by the integral value of the electron-phonon coupling constant $\lambda$.

For strongly hole doped bulk Bi$_2$Te$_3$ ($p = 8 \times 10^{20} \text{ cm}^{-3}$, c.f. Fig. 4, dotted lines) the coupling constant was estimated from the Debye temperature$^{50}$ via the McMillan formula$^{51}$ to be $\lambda \approx 0.62$. However, for smaller, thermoelectric feasible, charge carrier concentrations (in the order of a few $10^{19} \text{ cm}^{-3}$) the coupling constant was very recently extracted from ARPES measurements$^{52}$. Very small bulk contributions of about $\lambda \approx 0.05$ ($\lambda \approx 0.17$) were found for p-doped (n-doped) samples$^{52}$ (c.f. Fig. 4, solid and dashed lines, respectively). The electron-phonon coupling of the surface state is known to be very weak as well. Here, for Bi$_2$Te$_3$ values of $\lambda_{SS} \approx 0.05$ could be revealed experimentally$^{52}$ and theoretically$^{53,54}$. These findings go along with previous similar results for the topological insulator Bi$_2$Se$_3$ ($\lambda_{SS} \approx 0.076 \ldots 0.088$)$^{55}$. To shed some light on the possible influence of electron-phonon coupling to the total relaxation time, the latter is depicted in Fig. 4 for the previously described scenarios of the electron-phonon coupling parameter $\lambda$.

With the depicted dependence of $\tau_{tot}$ and $\tau_{el-ph}$, it is obvious that electron-phonon processes will not noticeably contribute to thermoelectric electron transport at room-temperature and below, as the electron-phonon scatter-
FIG. 4. (color online) Electron-phonon contribution (red lines) to the temperature-dependent total relaxation time (black lines) of Bi$_2$Te$_3$ for different charge carrier concentrations and values of the integral electron-phonon coupling parameter $\lambda$. Further description within the text.
\[
\int_{\mu_{\text{max}}}^{\mu_{\text{min}}} \text{d}E g(E)[f(\mu, T) - 1] + \int_{\mu_{\text{min}}}^{\mu_{\text{max}}} \text{d}E g(E)f(\mu, T).
\]

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