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Optical conductivity of topological insulator thin films

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We present a detailed theoretical study on the optoelectronic properties of topological insulator thin film (TITFs). The $k \cdot p$ approach is employed to calculate the energy spectra and wave functions for both the bulk and surface states in the TITF. With these obtained results, the optical conductivities induced by different electronic transitions among the bulk and surface states are evaluated using the energy-balance equation derived from the Boltzmann equation. We find that for Bi$_2$Se$_3$-based TITFs, three characteristic regimes for the optical absorption can be observed. (i) In the low radiation frequency regime (photon energy $h\omega < 200$ meV), the free-carrier absorption takes place due to intraband electronic transitions. An optical absorption window can be observed. (ii) In the intermediate radiation frequency regime (200 $< h\omega < 300$ meV), the optical absorption is induced mainly by interband electronic transitions from surface states in the valence band to surface states in the conduction band and an universal value $\sigma_0 = e^2/(2h)$ for the optical conductivity can be obtained. (iii) In the high radiation frequency regime ($h\omega > 300$ meV), the optical absorption can be achieved via interband electronic transitions from bulk and surface states in the valence band to bulk and surface states in the conduction band. A strong absorption peak can be observed. These interesting findings indicate that optical measurements can be applied to identify the energy regimes of bulk and surface states in the TITF. © 2015 AIP Publishing LLC.

I. INTRODUCTION

In recent years, owning to their exotic electronic properties, topological insulators (TIs) have received a great attention in both the fields of condensed-matter physics and materials science.1–4 TI is a new state of quantum matter, which is characterized by an insulating bulk band-gap and gapless conducting edge or surface states. TI boundary (edge or surface) states protected by the time-reversal (TR) symmetry are topologically robust against TR-invariant disorders, and their spin orientations are strictly determined by their momentum directions due to the spin-momentum lockage.1,2 Therefore, these states can carry spin-polarized dissipationless currents, making TIs find potential applications in quantum computation and spintronic devices.

Two-dimensional (2D) TIs with quantum spin Hall effect have been theoretically predicted and experimentally confirmed in CdTe/HgTe and InAs/GaSb quantum wells.5–8 Three-dimensional (3D) or bulk TIs such as Bi$_2$Se$_3$ and Bi$_2$Te$_3$ systems were theoretically predicted to have a bulk band-gap as large as 300 meV and a single Dirac cone with gapless surface states.9,10 Such linear-like energy spectrum has been observed experimentally by angle-resolved photo-emission spectroscopy.10,11 Moreover, TI thin films (TITFs) have also been fabricated with various material growth techniques such as molecular beam epitaxy (MBE),12 chemical vapor deposition,13 and mechanical exfoliation.14 With the decrease in thickness of the TITF, the electronic states at top and bottom surfaces can hybridize to open a finite gap in the surface-state energy spectrum, as theoretically predicted and experimentally verified.16 As a result, more interesting features of the physical properties can be observed in TITFs. For instance, it has been theoretically17 shown that due to the inter-surface coupling, the interesting spin-dependent properties of gapped surface states can be observed in TITFs, including the topological quantum phase transition, surface spin Hall effect, spin-dependent orbital magnetic moment, and spin-dependent optical transition selection rule. Very recently, it has been theoretically18 demonstrated that the inter-surface coupling can give rise to the reduction of the carrier group velocity and the breaking of the spin-momentum lockage in TITFs, and a combination of these two results can explain the experimental observation of the mobility reduction in TITFs as compared to bulk TIs.

At present, most of the research activities on TIs have been focused on their electronic and transport properties. Less research work has been carried out on their optical and optoelectronic properties. Recently, the optical conductivity/absorption induced by the interband optical transition among TI surface states was examined theoretically.19,20 It is known that the surface states are located in the relatively low energy regime in the energy spectrum of the TI (see Fig. 1(b)). As a result, the corresponding optical absorption only occurs in the relatively low radiation frequency regime (see ss channel in Fig. 1(b)). However, when the radiation photon energy is large enough so that it exceeds the bulk band-gap of the TI, the bulk states would take part in photon-induced electronic transition events. As a result, more transition channels open

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up for the optical absorption (see Fig. 1(b)) and more interesting features for the optical properties of the TI may be expected. When the radiation photon energy is large enough, four interband transition channels (see bs, bb, ss, and sb channels shown in Fig. 1(b)) make contributions to the optical absorption in the TI. On the other hand, like in conventional electronic systems, the free-carrier optical absorption can occur in low frequency regime due to intraband electronic transitions in the TI. Therefore, it is important and significant to examine the optical conductivity/absorption in the TI in a wider spectrum, especially in low and high frequency regimes, and it becomes the prime motivation of the present study.

In this work, we develop a theoretical approach to study optoelectronic properties induced by both the surface and bulk states in the TITF. The effective Hamiltonian derived from the k · p model is employed to calculate the energy spectra and wave functions for the bulk and surface states in the TITF. With these obtained results, the optical conductivity for the corresponding system is evaluated using the energy-balance equation derived from the Boltzmann equation. We intend to examine how surface and bulk carriers in the TITF respond to the applied radiation field and how different electronic transition channels can affect the optical conductivity/absorption in the TITF. This paper is organized as follows. In Sec. II, the theoretical approach is developed to calculate the electronic band structure and optical conductivity of the TITF. The main theoretical results are presented and discussed in Sec. III. Finally, the concluding remarks are summarized in Sec. IV.

II. THEORETICAL APPROACH

In the present work, we consider a TITF grown along the z-direction and placed on a dielectric substrate (see Fig. 1(a)). The thickness of TITF is L and the top (bottom) surface locates at $z = L/2$ and $z = -L/2$. It is known that the surface states in the TI can be described simply by the Dirac-type Hamiltonian. However, there is no simple analytical results for the bulk states in the TI. The most tractable theoretical approach to include both bulk and surface states in the calculation is through the $k \cdot p$ method. In the four basis $|P1^+_z, \uparrow⟩$, $|P2^-_z, \downarrow⟩$, $|P1^-_z, \downarrow⟩$, and $|P2^+_z, \downarrow⟩$, with the superscripts $±$ standing for even and odd parities and $\uparrow (\downarrow)$ for spin up (down) of an electronic state, the effective Hamiltonian derived from the $k \cdot p$ model for bulk and surface states in the TI can be written as

$$H = \begin{bmatrix} M(K) & A_1 k_z & 0 & A_2 k_- \\ A_1 k_z & -M(K) & A_2 k_+ & 0 \\ 0 & A_2 k_+ & M(K) & -A_1 k_z \\ A_2 k_+ & 0 & -A_1 k_z & -M(K) \end{bmatrix} + C(K)I_4,$$

where $K = (k_x, k_y, k_z)$ is the electron wavevector, $k_\pm = k_x \pm ik_y$, $C(K) = C_0 + C_1 k_x^2 + C_2 (k_y^2 + k_z^2)$, $M(K) = M_0 + M_1 k_x^2 + M_2 (k_y^2 + k_z^2)$, $I_4$ is a 4 × 4 identity matrix, and $A_i$ ($i = 1, 2$, $C_i$ ($i = 0, 1, 2$), and $M_i$ ($i = 0, 1, 2$) are materialspecific parameters. It has been demonstrated that this Hamiltonian can be applied to describe the bulk and surface states in bulk TIs such as Bi$_2$Te$_3$ and Bi$_2$Se$_3$ systems. For the TITF system, $k_x$ and $k_y$ are good quantum numbers due to translational symmetry in the ($x, y$)-plane, while $k_z$ is no longer a good quantum number since the TI film is thin in the $z$-direction. Therefore, the model Hamiltonian for TITF can be obtained via making the substitution $k_z \rightarrow -i\partial/\partial z$ in Eq. (1). This is the spirit of envelope function theory applied to deal with the problem of electronic states in low-dimensional nanostructures. The energy spectra and wave functions for bulk and surface states in the TITF are obtained from the following Schrödinger equation:

$$H \Psi = E \Psi,$$

where $E$ is the carrier energy and $\Psi$ is the carrier wave function. We use the finite difference method$^{23}$ to numerically solve this Schrödinger equation.

We now consider a radiation field applied perpendicular to the ($x, y$)-plane of TITF and assume it is polarized linearly along the $x$-direction, as illustrated in Fig. 1(a). The carrier-photon (cp) interaction Hamiltonian in the TITF can be obtained by replacing $k$ with $k + eA/t$ with $A$ being the vector potential of radiation field, which reads

$$H_{cp} = \frac{eA_x}{\hbar} \begin{bmatrix} D_+ k_x & 0 & 0 & A_x \\ 0 & 0 & 0 & A_x \\ A_x & 0 & D_- k_x & 0 \\ 0 & A_x & 0 & D_- k_x \end{bmatrix},$$

where $D_\pm = 2(C_\pm M_2)$, $A_x = (A_x, 0)$, and $A_x = (F_0/\omega) \sin \omega t$ with $F_0$ and $\omega$ being the electric field strength and frequency of radiation field, respectively. In the derivation of Eq. (3), we limit ourselves to the case of a weak radiation field so that the contribution from the $F_0^2$ term can be neglected. It
should be noted that the carrier-photon interaction Hamiltonian can also be expressed as

$$H_{cp} = \frac{eA_\nu}{\hbar} \frac{\partial H}{\partial k_x}$$  \tag{4}$$

under the weak field approximation.

Applying the wave function and energy spectrum obtained from solving Eq. (2) into Fermi’s golden rule, the steady-state electronic transition rate induced by the carrier-photon interaction in the TITF can be obtained as

$$W_{x\lambda}^{c\xi}(k,k') = \sigma_{x\lambda}(\epsilon_k) \delta_{k,k'},$$

where

$$W_{x\lambda}^{c\xi}(k) = \frac{2\pi}{\hbar} \left( \frac{eF_0}{\hbar c} \right)^2 \left| \left\langle \Psi_{x\lambda}^{c\xi}(k) \left| \frac{\partial H}{\partial k_x} \right| \Psi_{x\lambda}^{c\xi}(k) \right\rangle \right|^2 \times \delta \left[ E_{x\lambda}^{c\xi}(k) - E_{x\lambda}^{c\xi}(k) - \hbar \omega \right].$$ \tag{5}$$

Here, $\xi$ refers to the conduction or valence band and $\lambda$ to the surface or bulk state in the conduction or valence band, $\Psi_{x\lambda}^{c\xi}(k)$ is the carrier wave function, and $E_{x\lambda}^{c\xi}(k)$ is the carrier energy. To better understand the meaning of indices $\xi$ and $\lambda$, and in the transition regime, it is necessary to make following statements: For the TITF considered in the present study, the conduction band refers to the energy regime above the gapped Dirac point and the valence band to the energy regime below the gapped Dirac point. Since the electronic states are divided into the surface and bulk states in the TITF, both the conduction and valence bands include two spin-degenerate branches of the surface states and many spin-degenerate branches of the bulk states. Thus, we employ $\xi$ to denote the conduction or valence band and $\lambda$ to the surface or bulk state in the conduction or valence band.

With the steady-state electronic transition rate, we can employ the Boltzmann equation to study the optical response of carriers in bulk and surface states in the TITF. In the case of degenerate statistics, the Boltzmann equation for bulk and surface carriers in the TITF takes a form

$$\frac{\partial f_{x\lambda}^{c\xi}(k,t)}{\partial t} = \sum_{\xi',\lambda'} F_{x\lambda\xi'}(k',t) - F_{x\lambda\xi'}(k,k',t).$$ \tag{6}$$

Here, $F_{x\lambda\xi'}(k,k',t) = f_{x\lambda}^{c\xi}(k,t) \left[ 1 - f_{x\lambda}^{c\xi}(k',t) \right] W_{x\lambda\xi'}^{c\xi}(k,k'),$ and $f_{x\lambda}^{c\xi}(k,t)$ is the momentum-distribution function for an electron at a state $|\xi',\lambda,k\rangle$ at time $t$. In Eq. (6), the effect of the radiation field has been included within the time-dependent carrier distribution function and within the electronic transition rate. Thus, to avoid double counting, the force term induced by the radiation field does not appear on the left-hand side of the Boltzmann equation. It is known that there is no simple and analytical solution to Eq. (6) with the electronic transition rate given by Eq. (5). In this work, we apply the usual balance-equation approach to solve the problem.23

By multiplying $\sum_{\xi,\lambda,k} E_{\lambda}^{c\xi}(k)$ to both sides of Eq. (6), we can derive the so-called energy-balance equation. From it, the electron energy-transition rate induced by the carrier-photon interaction is obtained as: $P = \hbar \omega/\tau$, where

$$\tau^{-1} = \sum_{\xi' \lambda' \lambda, k} f_{x\lambda}^{c\xi}(k) \left[ 1 - f_{x\lambda}^{c\xi}(k') \right] W_{x\lambda\xi'}^{c\xi}(k) \tag{7}$$

with $\tau$ being the energy relaxation time, and $P = \sum_{\xi' \lambda' \lambda, k} E_{\lambda}^{c\xi}(k) \partial f_{x\lambda}^{c\xi}(k,t)/\partial t$ is the electronic energy-transfer rate per surface area in the TITF. Here, we have used a statistical energy distribution such as the Fermi-Dirac function as carrier distribution function at a steady state. Namely, we have taken $f_{x\lambda}^{c\xi}(k,t) \approx f_{x\lambda}(E_{\lambda}^{c\xi}(k))$, where $f_{x\lambda}(x) = \left[ e^{(x-\mu)/kT} + 1 \right]^{-1}$ is the Fermi-Dirac function, with $\mu$ being the chemical potential for electrons or holes in the TITF. The optical conductivity induced by the carrier-photon interaction can be calculated through\textsuperscript{24}

$$\sigma(\omega) = P/F_0^2 = \sum_{\xi' \lambda' \lambda, \omega} \sigma_{x\lambda}(\omega), \tag{8}$$

where $\sigma_{x\lambda}(\omega)$ is the optical conductivity induced by the electronic transition from surface or bulk states (labeled by $\lambda$) in $\xi$ band to surface or bulk states (labeled by $\lambda'$) in $\xi'$ band. We note that the electron transition cannot be achieved from higher-energy surface or bulk states in the conduction band to low-energy surface or bulk states in the valence band via the optical absorption scattering. Thus, $\sigma_{x\lambda}(\omega) = 0$, where the notations $C$ and $V$ denote the conduction and valence bands, respectively. Since the overlap of bulk-state and surface-state wave functions in the same conduction or valence band is very small, the electronic transition between bulk and surface states cannot be achieved strongly in the same conduction or valence band. Thus, $\sigma_{x\lambda}(\omega) = \sigma_{x\lambda'}(\omega) = 0$. After defining $\sigma_{x\lambda}(\omega) = \sigma_{x\lambda'}(\omega)$ induced by the interband transition and $\sigma_{x\lambda}(\omega) = \sigma_{x\lambda'}(\omega)$ induced by the intraband transition, we have

$$\sigma(\omega) = \sum_{\lambda} \left[ \sigma_{C\lambda}(\omega) + \sigma_{V\lambda}(\omega) \right] + \sum_{\lambda, \lambda'} \sigma_{x\lambda}(\omega). \tag{9}$$

This equation included the following contribution terms to the total optical conductivity: $\sigma_{x\lambda} (\sigma_{x\lambda'})$ induced by the intraband transition among surface (bulk) states in the same conduction band, $\sigma_{y\lambda} (\sigma_{y\lambda'})$ by the intraband transition among surface (bulk) states in the same valence band, $\sigma_{x\lambda} (\sigma_{y\lambda'})$ by the interband transition from surface (bulk) states in the valence band to surface (bulk) states in the conduction band, and $\sigma_{x\lambda} (\sigma_{y\lambda'})$ by the interband transition from surface (bulk) states in the valence band to bulk (surface) states in the conduction band. These contribution terms are induced by different optical transition channels, as shown in Fig. 1(b).

In the present study, we calculate the optical conductivities induced by different transition channels numerically because carrier wave function and energy spectrum are obtained numerically. In the numerical calculation, the $\delta$-function appearing in the electronic transition rate given by Eq. (5) is replaced by the normalized Gaussian distribution.25
\[ \delta \left[ \Delta_{\mathbf{k}}^{\mathcal{L}}(\mathbf{k}) - \hbar \omega \right] = \frac{1}{\sqrt{2\pi}} \exp \left( - \frac{\left[ \Delta_{\mathbf{k}}^{\mathcal{L}}(\mathbf{k}) - \hbar \omega \right]^2}{2\Gamma^2} \right), \]

where \( \Delta_{\mathbf{k}}^{\mathcal{L}}(\mathbf{k}) = E_{\mathbf{k}}^{\mathcal{L}}(\mathbf{k}) - E_{\mathbf{k}}^{\mathcal{L}}(\mathbf{k}) \) and \( \Gamma \) is the energy broadening factor due to various scattering mechanisms.

### III. RESULTS AND DISCUSSIONS

In this work, we consider Bi\(_2\)Se\(_3\)-based TITFs. It has been shown that the thickness of the TITF can reach down to few quintuple layers (QLs, 1 QL \( \approx 1 \) nm) via MBE growth of Bi\(_2\)Se\(_3\) layers on the thick sapphire substrate (Al\(_2\)O\(_3\)).\(^{26}\)

For the band structure calculation, the model parameters \( A_i \) \((i = 1, 2)\), \( C_i \) \((i = 0, 1, 2)\), and \( M_i \) \((i = 0, 1, 2)\) for Bi\(_2\)Se\(_3\) are taken from the first-principle calculation.\(^9\)

In Fig. 2, we show the energy spectra for the bulk and surface states in the TITF with different thicknesses \( L = 4 \) nm in panel (a), \( L = 6 \) nm in (b), and \( L = 8 \) nm in (c). From this figure, we can observe the following interesting features. (1) A quantum-well subband structure is formed for the bulk states in both conduction and valence bands due to quantum-confinement effect. The energy separations between different subbands for the bulk states in both conduction and valence bands increase with the decrease in thickness of the TITF. As a result, the number of bulk subbands is reduced with decreasing \( L \). (2) The bulk band-gap \( (E_b^b) \) of the TITF depends sensitively on thickness of the TITF. For instance, \( E_b^b \) is about 559 meV for a thicker TITF with \( L = 8 \) nm, while it is 625 meV for a thinner TITF with \( L = 4 \) nm. We notice that \( E_b^b \) is 100–300 meV for bulk TIs such as Bi\(_2\)Te\(_3\) and Bi\(_2\)Se\(_3\). Hence, the quantum-confinement effect makes the bulk band-gap of the TITF significantly larger than that of bulk TI. (3) The bulk-state energy spectrum in the TITF is generally non-parabolic, especially for bulk subbands in the valence band which may show a two-peak structure and the maximum energy may not appear at \( k = 0 \). (4) As expected, the surface states lie inside the bulk band-gap of the TITF and the surface-state energy spectrum exhibits a linear-like behavior around the zone center \( k = 0 \).

With reducing thickness of the TITF, a finite gap can be induced in the surface-state energy spectrum (see Fig. 2(a)). This surface gap is formed due to hybridization between top and bottom surface states in the TITF.

The effect of surface-state hybridization can be demonstrated more clearly with probability density distributions of the surface states, as shown in Fig. 3. We see clearly that with the decrease in thickness of the TITF, the surface states at top and bottom surfaces can couple (hybridize) substantially. It should be noted from Fig. 3 that the surface states are mainly located near two surfaces of the TITF. It is known that the bulk states are mainly located around the center of the TITF. This verifies our previous approximation that the strength of the intraband electronic transition between bulk and surface states is rather weak due to the very small overlap of surface-state and bulk-state wave functions. These interesting features can play a vital role in understanding the optoelectronic properties induced by surface and bulk states in the TITF.

For the numerical calculation on the optical conductivity of the TITF, we consider the conducting carriers in the system are electrons. If \( N_0 \sim 10^{17} - 10^{18} \) cm\(^{-3}\) is the electron density in the absence of radiation field (i.e., the dark electron density), the electron density in the presence of light radiation is given by \( N_e = N_0 + \Delta N_e \), where \( \Delta N_e \sim 10^{17} \) cm\(^{-3}\) is the photo-induced electron density. Under the condition of charge number conservation, \( N_e = \Delta N_e \) is the hole density in the presence of the radiation field. At a finite temperature, the chemical potentials \( \mu_e \) and \( \mu_h \) for electrons and holes in a TITF sample can be determined, respectively, through

\[ N_e = \frac{1}{L} \sum \int \mathcal{E}_{\mathbf{k}}^{c} f_{\mathbf{k}} \]

and

\[ N_h = \frac{1}{L} \sum \int (1 - f_{\mathbf{k}}) \mathcal{E}_{\mathbf{k}}^{c} \].

![Fig. 2. Energy spectra of bulk and surface states in the TITF for different thicknesses: (a) \( L = 4 \) nm, (b) \( L = 6 \) nm, and (c) \( L = 8 \) nm. Here, the red and blue curves represent the bulk and surface states, respectively.](image1)

![Fig. 3. Probability density distributions of surface states in the conduction band in the TITF for different thicknesses \( L \) as indicated. The results shown here are plotted at the zone center \( k = 0 \).](image2)
In general, the photo-induced carrier density depends on the radiation intensity and frequency and on other scattering and relaxation mechanisms. In the present study, we assume that the photo-excited carrier density is about $N_e = n_e = 10^{17}$ cm$^{-3}$. Furthermore, the electronic energy broadening is assumed to be $\Gamma = 10$ meV, which corresponds to a picosecond-scale energy relaxation time induced by electronic scattering mechanisms in the TITF.

In Fig. 4, we show contributions from different electronic transition channels to the optical conductivity of the TITF at the fixed film thickness $L$, temperature $T$, and electron density $N_e$. In the TITF, the optical conductivity or absorption is mainly induced by interband ($\sigma_{ib}$) and intraband ($\sigma_{ib}$ and $\sigma_{is}$) electronic transition channels, as shown in Fig. 4. From this figure, we notice three characteristic regimes for the optical conductivity or absorption. (i) Like in conventional electronic systems, in the low radiation frequency regime (photon energy $\hbar \omega < 200$ meV), the optical conductivity is mainly induced by the free-carrier absorption achieved via intraband transitions among surface states in both the conduction and valence bands in the TITF. In the n-type TITF, because the hole states are mainly induced by optical pumping, the transition channels between surface states in the valance band are not as many as those in the conduction band. Thus, $\sigma_{ib} = \sigma_{ib}$ is much larger than $\sigma_{is}(\omega)$, as shown in Fig. 4. Here, we have considered a situation where the chemical potentials for electrons and hole are located inside the bulk band-gap of the TITF. As a result, $\sigma_{ib}(\omega) \approx \sigma_{is}(\omega) \approx 0$. The optical conductivity induced by free-carrier absorption in the TITF increases with decreasing the radiation frequency, similar to that in conventional electronic systems. In this frequency regime, the optical conductivity can also be induced by interband transition channels among the surface states, $\sigma_{is}$, as shown in Fig. 4. It gives rise to a cut-off of the optical absorption in this frequency regime. Therefore, an optical absorption window can be observed, which is induced by different transition energies required for interband and intraband optical absorptions. Similar optical absorption window was observed for graphene in the experimental and theoretical work.$^{27}$ (ii) In the intermediate radiation frequency regime ($200 < \hbar \omega < 300$ meV), the optical absorption is dominated by interband transitions from surface states in the valance band to surface states in the conduction band. A universal value $\sigma_\infty = e^2/(8\hbar)$ for the optical conductivity can be observed in this radiation frequency regime. Such a universal optical conductivity is a consequence of linear-like energy spectrum for the surface states in the TITF. Similar effect has been demonstrated for graphene. It should be noted that the universal optical conductivity of the TITF is just a half of the value $\sigma = e^2/(4\hbar)$ observed for the graphene.$^{27}$ (iii) In the high radiation frequency regime ($\hbar \omega > 300$ meV), the optical absorption can be achieved via interband transitions from bulk and surface states in the valance band to bulk and surface states in the conduction band. In this frequency regime, the optical conductivity first increases because of opening up of interband transition channels from bulk states in the valence band to surface states in the conduction band as well as from surface states in the valence band to bulk states in the conduction band, and then a strong absorption peak can be observed due to interband transitions from bulk states in the valence band to bulk states in the conduction band. We note that $\sigma_{bb}(\omega)$ is much larger than $\sigma_{ib}(\omega)$ and $\sigma_{is}(\omega)$. Hence, the optical absorption peak corresponds to the energy gap between conduction and valence bands for the bulk states. This means that the bulk band-gap of the TITF $E_b$ can be measured directly via optical experiments. The major difference between optical conductivities of the TITF and graphene is that in the TITF the universal optical conductivity can only be observed in the mid-infrared spectral range, while in the graphene, it can stably exist in the infrared-to-visible spectral range.$^{28}$ This is because in the TITF, the bulk states play a key role in the optical conductivity at higher photon energies while such states are absent in the graphene.

In Fig. 5, we show temperature dependence of the optical conductivity of the TITF at the fixed thickness $L$ and electron densities $N_e$. At relatively low temperatures, the optical conductivity in the low radiation frequency regime

![FIG. 4. Contributions from different transition channels ($\sigma_{ib}$ and $\sigma_{is}$) to the optical conductivity of the TITF at the fixed thickness $L$, temperature $T$, and electron density $N_e$, as indicated. Here, the black solid curve represents the total optical conductivity and $\sigma_0 = e^2/(8\hbar)$.
](https://example.com/figure4.png)

![FIG. 5. Optical conductivity of the TITF at the fixed thickness $L$ and electron density $N_e$ for different temperatures $T$.
](https://example.com/figure5.png)
mainly via exciting of electrons from lower-energy occupied states to the higher-energy empty states and the chemical potential for electrons increases with increasing electron density, the number of intraband and interband transition channels decreases with increasing electron density. Therefore, the overall optical conductivity induced by these transition channels decreases with increasing electron density. This means that a deeper optical absorption window can be observed for a TITF sample with larger electron density. In the intermediate radiation frequency regime (200 < ℏω < 300 meV), the optical conductivity is mainly induced by the interband electronic transition from the surface states in the valence band to surface states in the conduction band and has an universal value σ₀, which is independent of electron density due to linear-like nature of surface-state energy spectrum. In the relatively high radiation frequency regime (ℏω > 300 meV), the optical conductivity depends weakly on electron density. This is because for the electron and hole densities given here, the chemical potentials for electrons and holes are both located inside the bulk band-gap of the TITF. Therefore, the interband optical transitions induced by the bulk states in this frequency regime are nearly unaffected by electron density. It should be pointed out that for a gate-controlled TITF placed on a dielectric substrate such as Al₂O₃ or SiO₂, a finite electron (hole) density can be induced in the TITF system by the positive (negative) gate voltage. By doing so, the electron (hole) density in the TITF structure can be tuned by the gate voltage. Thus, the corresponding optoelectronic properties of the device system can be electrically controlled.

In Fig. 7, we show the optical conductivity of the TITF for different film thicknesses L at the fixed temperature T and electron density Nₑ. In the low radiation frequency regime (ℏω < 300 meV), the optical conductivity induced by free-carrier (intraband) absorption and interband absorption by surface states increases with decreasing thickness of the TITF, leading to some deviation from its universal value σ₀ in the intermediate radiation frequency regime (200 < ℏω < 300 meV). The enhanced optical conductivity in this frequency regime can be understood as follows. With the decrease in thickness of the TITF, the electronic states at top and bottom surfaces can hybridize to open a finite gap in
the surface-state energy spectrum (see Figs. 2 and 3). As a result, both strengths of intraband and interband electronic transitions among the surface states can be enhanced by this surface gap due to improved wave-function overlap of gapped surface states. However, in the high radiation frequency regime ($h\omega > 300$ meV), the optical conductivity decreases with decreasing thickness of the TITF. The explanation for the decrease of optical conductivity in this frequency regime is below. As thickness of the TITF decreases, the number of bulk subbands is reduced due to the quantum-size effect (see Fig. 2). Thus, the number of interband transition channels among the bulk states is reduced so that the optical conductivity decreases with the decrease in thickness of the TITF.

Furthermore, the optical absorption peak in this frequency regime is blue-shifted since the bulk band-gap of the TITF increases with the decrease in thickness of the TITF due to the quantum-size effect.

IV. CONCLUDING REMARKS

In this paper, we have theoretically investigated the optoelectronic properties of the TITF. The effective Hamiltonian derived from the $k \cdot p$ model has been employed to calculate the energy spectra and wave function for both bulk and surface states in the TITF. With these obtained results, the optical conductivities induced by different electronic transition channels among the bulk and surface states have been evaluated using the energy-balance equation derived from the Boltzmann equation.

We have found that for Bi$_2$Se$_3$-based TITFs, three characteristic regimes for the optical absorption can be observed. (1) In the low radiation frequency regime (photon energy $h\omega < 200$ meV), the free-carrier optical absorption takes place due to intraband electronic transitions. An optical absorption window can be observed, which is induced by different transition energies required for interband and intraband optical absorption. (2) In the intermediate radiation frequency regime ($200 < h\omega < 300$ meV), the optical absorption is mainly induced by transitions from surface states in the valance band to surface states in the conduction band and an universal value $\sigma_0 = e^2/(8\hbar)$ for the optical conductivity can be observed. In this frequency regime, the optical conductivity depends little on temperature and electron density. This is due to linear nature of the surface-state energy spectrum in the TITF. Similar effect has been observed in graphene system. (3) In the high radiation frequency regime ($h\omega > 300$ meV), the optical absorption can be achieved via interband transitions from bulk and surface states in the valance band to bulk and surface states in the conduction band. A strong absorption peak can be observed. Therefore, the optical conductivity of the TITF differs markedly from graphene where the universal optical conductivity can be seen over a wide frequency regime from infrared to visible. Such a major difference is due to the presence of bulk states in the TITF which are absent in graphene. We have also examined the dependence of optical conductivity of the TITF on temperature, electron density, and film thickness. The obtained results demonstrate that optical measurements can be applied to identify the energy regimes of the bulk and surface states and to determine the bulk band-gap of the TITF. These interesting findings indicate that optical measurements can be applied to identify the energy regimes of bulk and surface states in the TITF and that TITFs can be applied not only as electronic and thermal electronic devices but also as practical optoelectronic devices.

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