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Qinjun Chen

University of Wollongong, qc691@uowmail.edu.au

Yee Sin Ang

University of Wollongong, ysa190@uowmail.edu.au

Xiaolin Wang

University of Wollongong, xiaolin@uow.edu.au

R A. Lewis

University of Wollongong, roger@uow.edu.au

Chao Zhang

University of Wollongong, czhang@uow.edu.au

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Abstract

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Keywords

quantum, cdte, hgte, wells, rate, loss, particle, charged, energy

Disciplines

Engineering | Science and Technology Studies

Publication Details

Chen, Q., Ang, Y., Wang, X., Lewis, R. A. & Zhang, C. (2013). Energy loss rate of a charged particle in HgTe/(HgTe, CdTe) quantum wells. *Applied Physics Letters*, 103 192107-1-192107-3.

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Citation: [Applied Physics Letters](#) **103**, 192107 (2013); doi: 10.1063/1.4829467

View online: <http://dx.doi.org/10.1063/1.4829467>

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Energy loss rate of a charged particle in HgTe/(HgTe, CdTe) quantum wells

Qinjun Chen,¹ Yee Sin Ang,¹ Xiaolin Wang,² R. A. Lewis,^{1,2} and Chao Zhang^{1,2,a)}

¹School of Physics, University of Wollongong, New South Wales 2522, Australia

²Institute for Superconducting and Electronic Materials, University of Wollongong, New South Wales 2522, Australia

(Received 1 October 2013; accepted 24 October 2013; published online 6 November 2013)

The energy loss rate (ELR) of a charged particle in a HgTe/(HgTe, CdTe) quantum well is investigated. We consider scattering of a charged particle by the bulk insulating states in this type of topological insulator. It is found that the ELR characteristics due to the intraband excitation have a linear energy dependence while those due to interband excitation depend on the energy exponentially. An interesting quantitative result is that for a large range of the incident energy, the mean inelastic scattering rate is around a few terahertz. © 2013 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4829467>]

HgTe/(Cd, Hg)Te quantum well (QW) topological insulators have attracted intense attention due to its strong spin orbit coupling and band inversion when its thickness is increased beyond the critical value ($d_c = 6.3$ nm).^{1–8} It is well known that HgTe has an intrinsic band gap of -0.3 eV playing the role as well material, while CdTe has a positive gap of 1.6 eV building up a barrier for the well electrons.^{1–3} With increasing the thickness of HgTe/(Cd, Hg)Te QW up to above 6.3 nm, the heavy Hg ions in the “well” pull the s -like Γ_6 band down below the p -like Γ_8 band, giving rise to an inverted band structure, which is beneficial for tuning band-gaps (from 0 to 1.6 eV).¹ Consequentially, HgTe/(Cd, Hg)Te QWs exhibit many interesting features, such as large Rashba spin-orbit splitting effect,⁴ quantum Andreev effect,⁵ and weak anti-localization effect.⁶ Recently, by taking advantage of the molecular beam epitaxy technique, HgTe/(Cd, Hg)Te QWs were first designed as two dimensional (2D) topological insulator (TI).^{7,8} In this system, a gapless band structure was generated on the sample edge due to the strong spin-orbit interaction and significant band inversion. However, a finite band gap remains in the two dimensional bulk states.^{7,8} This unique feature restricts electrons motion in the forward direction due to the interlocking its spin and momentum. The forward motion is topologically protected from nonmagnetic impurity scattering due to the time reversal symmetry.⁹ So far, quantum spin Hall effect,^{7,8} as well as the non-local transport on the edge state without applying a magnetic field,¹⁰ has been observed in the low carrier density and high electron mobility HgTe/(Cd, Hg)Te TIs. These studies have suggested that HgTe/(Cd, Hg)Te QWs could be the candidate for the next generation “spintronics” technology. This type of TI QW has also been shown to be an efficient photomixer in terahertz regime.¹¹

Electron energy loss spectroscopy (EELS) has been a very useful probe of materials properties. In EELS, the interaction between a charged external particle and an electronic system has been employed to reveal electron excitations in condensed matter physics and nuclear.^{12–15} The scattering cross section of an external particles by an electronic system can be directly related to the density-density

correlation function, the screening properties, and the inter-particle coupling. In moving through an electronic system, the charged particle experiences both momentum and energy loss due to the nature of the inelastic scattering. For an n -type HgTe/(Cd, Hg)Te QWs, 2DEG is confined in the well with a gap of the bulk states related to the well thickness. The scattering of an external charged particle in the system can be by both the gapless edge states as well as the gapped bulk states.

In this paper, we study the energy loss rate of an external electron in the n -type HgTe/(Cd, Hg)Te QWs. We consider a process of an incoming particle of momentum $\mathbf{p}$ and energy $\varepsilon_{\mathbf{p}} = \hbar^2 \mathbf{p}^2 / 2m$, interacting with the HgTe/(Cd, Hg)Te QW through a screened Coulomb interaction $g_{\mathbf{q}}$. The momentum transfer and the energy loss in a scattering are $\mathbf{q}$ and $\omega = \varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}-\mathbf{q}} = pq \cos \theta / m - q^2 / 2m$, respectively, where θ is the angle between $\mathbf{p}$ and $\mathbf{q}$. The energy loss rate of a particle in a two dimensional system is typically defined as

$$\frac{d\varepsilon_{\mathbf{p}}}{dt} = \int \frac{d^2 \mathbf{q}}{(2\pi)^2} W_{\mathbf{q}}(\omega) [\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}-\mathbf{q}}], \quad (1)$$

where $W_{\mathbf{q}}(\omega)$ is the transition probability, which is given by

$$W_{\mathbf{q}}(\omega) = 2 \frac{g_{\mathbf{q}}}{1 - e^{-\beta\omega}} \text{Im} \left[\frac{1}{\kappa_{\mathbf{q}}(\omega)} \right], \quad (2)$$

$\beta = 1/k_B T$ with k_B is the Boltzmann constant. $g_{\mathbf{q}}$ is the coupling constant describing the interaction between the incident electron and 2D electrons trapped in the “well.” Here, 2D screened Coulomb potential was adopted as the expression of $g_{\mathbf{q}}$, which is of the form¹⁶

$$g_{\mathbf{q}} = \frac{1}{q + q_s}. \quad (3)$$

Here, q_s is the screening wavenumber, $q_s = \frac{m^* e}{2\pi \hbar^2 \kappa_s} (1 - e^{-\frac{\hbar^2 \beta \pi n}{m^*}})$, where m^* is the effective mass of electron, n is the carrier density of HgTe/(Cd, Hg)Te QW, which is self-consistent with chemical potential, and κ_s is the electric constant of the material. In the above expression, we have only included the scattering by the particle-hole excitation, assuming that the plasmon of

^{a)}czhang@uow.edu.au

the gapless states is heavily damped and the inter-band plasmon is at a much higher energy.

The dielectric function of the QW can be obtained from the electronic properties. The Hamiltonian of a HgTe/(Cd, Hg)Te QW can be written using the BHZ model,⁷

$$H(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & 0 \\ 0 & h^*(-\mathbf{k}) \end{pmatrix}, \quad (4)$$

$$h(\mathbf{k}) = G(\mathbf{k})\mathbf{I}_{2 \times 2} + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (5)$$

where $\mathbf{I}_{2 \times 2}$ is the 2 identity matrix, σ^a is the Pauli spin matrix, $G(\mathbf{k}) = C - D(k_x^2 + k_y^2)$, $d_x(\mathbf{k}) = Ak_x$, $d_y(\mathbf{k}) = -Ak_y$, and $d_z(\mathbf{k}) = M(\mathbf{k})$, and $M(\mathbf{k}) = M - B(k_x^2 + k_y^2)$. A, B, C, D, and M are parameters determined by the material geometry. The values of these parameters for a QW of thickness 7.0 nm are given in Ref. 7: $A = 0.3645 \text{ eV} \cdot \text{nm}$, $B = -0.686 \text{ eV} \cdot \text{nm}^2$, $D = -0.512 \text{ eV} \cdot \text{nm}^2$, and $M = -0.010 \text{ eV}$. And we shall use these values in our calculation. The energy dispersion relation is

$$E_{(s=\pm)} = C - Dk^2 + s\sqrt{(M - Bk^2)^2 + A^2k^2}. \quad (6)$$

The dynamical polarization function in the random-phase approximation is expressed as¹⁷

$$\Pi(\mathbf{q}, \omega) = \frac{g}{4\pi^2} \int d^2k \sum_{s,s'=\pm} F^{ss'}(\mathbf{k} + \mathbf{q}, \mathbf{q}) \frac{f_{\mathbf{k},s} - f_{\mathbf{k}+\mathbf{q},s'}}{E_{\mathbf{k},s} - E_{\mathbf{k}+\mathbf{q},s'} + \omega}, \quad (7)$$

where $F^{ss'}(\mathbf{k} + \mathbf{q}, \mathbf{q}) = |\varphi_{\mathbf{k},s}| |\varphi_{\mathbf{k}+\mathbf{q},s'}|^2$ is the wave-function overlap factor, $f_{\mathbf{k},s}$ is the Fermi-Dirac distribution, $E_{\mathbf{k},s}$ is the energy dispersion relation given above, and $\omega = \omega + i\delta (\delta \rightarrow 0)$. The dielectric function is written as $\kappa_q(\omega) = 1 - v_q \Pi(q, \omega)$, where $v_q = e^2/(\kappa_0 q)$ is the Fourier transformed electron-electron interaction.

In the following, we shall use the static approximation on the real part dielectric function by taking $\omega = 0$. The upper limit of the q -integration is $2p$, which is the maximum allowed momentum transfer in a scattering. Thus the integral is rewritten as

$$\begin{aligned} \frac{d\epsilon_p}{dt} &= \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2p} dq d\theta \frac{q}{1 - e^{-\beta\omega}} [2pq \cos \theta - q^2] \\ &\times g_q \left[\frac{v_q \text{Im}\Pi(q, \omega)}{|\kappa_q(\omega)|^2} \right]. \end{aligned} \quad (8)$$

In Fig. 1, we plot the momentum dependence of the energy loss rate (ELR) of an external electron in the n-type HgTe/(Cd, Hg)Te QW. The zero temperature chemical potential is chosen to be 0.05 eV. At low energy, the electron is only being scattered by the intraband excitations. For the present system, the band velocity is about $7 \times 10^5 \text{ m/s}$, and the electron effective mass is about $0.015 m_e$. For an incident electron with $p = \hbar(1/\text{nm})$, there is a large mismatch between the momentum of the incoming particle and that of the band electron. Therefore, the incoming electron loses very little energy to the intraband excitation of the QW. When this incident energy exceeds the threshold energy, which is the sum

FIG. 1. Momentum dependent ELR of an incident electron at 0 K and 77 K. We set $\hbar = 1$ here and after.

of the bandgap and the chemical potential, $\epsilon_{\text{th}} = E_g + \mu$ (corresponds to $p = \hbar(2.4/\text{nm})$), the electron can be strongly scattered by the interband excitations. As a result, the ELR increases significantly. The ELR by the intraband process and that by the interband process both increase with the incoming electron momentum. This is due to that the momentum transfer (or scattering phase space) increases with p . For the intraband process, the ELR is roughly quadratic in p . However, the ELR increases very rapidly with p at the onset of the interband process. When the incident energy reaches ϵ_{th} , the ELR resembles an exponential type of p -dependence. This suggests an activation-type electronic transition near the ϵ_{th} . At high momentum, all electronic excitations contribute to the energy and momentum exchange with the incoming particle and the ELR tends to saturate. This result is very different from non-doping cases, where ELR is dominated by the interband contribution.^{18,19}

The ELR from the intraband process increases with the temperature monotonically. As temperature increases, more carriers contribute to the static screening. As a result, the coupling between the incident particle and the quasiparticle excitations in the quantum well becomes stronger and ELR increases. Fig. 2 shows the temperature dependence of the ELR with incident momentum of $1.0/\text{nm}$ and $10/\text{nm}$ corresponding to the intraband process. At $p = 10/\text{nm}$, the ELR is mainly due to the interband process. The interband transition

FIG. 2. ELR versus temperature for external electrons with momenta $p = 1 \text{ nm}^{-1}$ and $p = 10 \text{ nm}^{-1}$.

FIG. 3. Mean inelastic scattering rate as a function of incident momentum at 0 K and 77 K.

FIG. 4. Diffusion constant normalized by $D_0 = D_{\max}(T=0)$ versus momentum of the incident electron at 0 K and 77 K.

rate decreases with the temperature due to the reduced phase space at high temperatures. This partly cancels the temperature effect of static screening. As a result, ELR is approximately temperature independent at high temperature and high momentum.

The mean inelastic scattering rate of the incident particle by the quantum is defined as $1/\tau = (d\varepsilon_p/dt)\varepsilon_p^{-1}$. Fig. 3 shows the mean scattering rate at zero temperature. For the intraband process, the scattering rate is nearly constant. There is a rapid increase in the rate near ε_{th} . At high momentum, the rate decreases with p . The interesting point is that for a large range of p , the scattering rate is between 1 and 5 terahertz. Therefore, it is expected that the ELR can be tuned resonantly by weak terahertz radiation.

We now briefly discuss another related physical quantity, the diffusion constant, defined as $D_p \sim (mp)^2 \tau_p \sim \varepsilon_p \tau_p$.

Fig. 4 shows the momentum dependent diffusion constant at zero temperature. The diffusion constant increases with the energy in the intraband excitation regime. There is a diffusion maximum when the incident energy is just below the threshold energy. When the sample size is in the order of mean free path, the particle can travel resonantly near the maximum diffusion. For a particle of incident velocity of 10^6 m/s and using the scattering rate given in Fig. 3, the estimated mean free path is around 10^{-3} m. This is comparable to typical sample sizes. The onset of the interband process leads to a sudden drop of D_p and a diffusion peak is observed at ε_{th} . For large momenta, D_p is approximately a quadratic function of the incoming momentum. For incoming energies immediately above ε_{th} , the diffusion is minimum in a finite range of p . This is quite intriguing, as it suggests that the incident electron is nearly localized due the strong scattering by the interband excitations.

In conclusion, the energy loss rate of an electron in an n-type HgTe/(Cd, Hg)Te QW has been calculated. We found that, for slow electrons, the ELR is determined by the intraband contribution only, while for fast electrons, the ELR is dominated by the interband contribution. The mean inelastic scattering rate is in the terahertz frequency regime. At different energies, the incident electron can either diffuse resonantly, or almost be localized.

This work was supported by the Australian Research Council (Grant No. DP 130102956).

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