

Supplementary Materials for “Warping effect-induced optical absorbance increment of topological insulator films for THz photodetectors with high signal-to-noise ratio”

J. M. Shao, H. Li, and G. W. Yang*

State Key Laboratory of Optoelectronic Materials and Technologies, Institute of Optoelectronic and Functional Composite Materials, Nanotechnology Research Center, School of Physics & Engineering, Sun Yat-sen University, Guangzhou 510275, Guangdong, P. R. China.

Calculations of SNR

This supplementary material is used to calculate the signal-to-noise ratio (*SNR*) of topological insulator (TI) films and bulk $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ photodetectors. It mainly follows the method used in the work of Zhang et al.¹ Unlike the main text, we restore $\hbar$ in this supplementary material.

For a photoresistor type photodetector, if the major noise is Johnson thermal noise, its *SNR* can be simply defined as the ratio of the photocurrent signal I_{ph} divided by the standard deviation of the thermal noise σ_{I_n} at temperature T . The photocurrent signal is $I_{ph} = 2e\eta pS/E_{ph}$ with e the electron charge, η the quantum efficiency, p the incident light power density, S the detecting area, E_{ph} the incident photon energy, and factor 2 for electron-hole pair. The standard deviation of the thermal noise is $\sigma_{I_n} = \sqrt{4k_B T \Delta f / R}$ with k_B the Boltzmann constant, Δf the bandwidth of the detector and R the resistance. So the *SNR* can be expressed as

$$SNR = \frac{I_{ph}}{\sigma_{I_n}} = \frac{2e\eta pS/E_{ph}}{\sqrt{4k_B T \Delta f / R}} = C\eta\sqrt{R} \quad (1)$$

where $C = \frac{2epS/E_{ph}}{\sqrt{4k_B T \Delta f}}$ is the material independent quantity, only related to the fundamental physical constants (like e and k_B) and the experimental condition parameters (like T and p). Thus, we get the basic fact that materials with higher quantum efficiency η and resistance R will have a better SNR . To allow sufficient absorption, we assume that the photon energy E_{ph} is much larger than the thermal energy $k_B T$ in the following discussion. And we use the non-degenerate assumption $E_{ph} = 6k_B T$ just like that in Ref. [1].

For three dimensional (3D) photodetecting material like $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$, $\eta = 1 - e^{-\beta l}$, $R = \rho \frac{l}{wt}$, where β is its absorption coefficient, l , w and t are its length, width and thickness, respectively. The resistivity ρ can be expressed using the intrinsic carrier density n_i along with the mobilities for electrons and holes, μ_e , μ_h

$$\rho = \frac{1}{en_i(\mu_e + \mu_h)}. \quad \text{\textbackslash* MERGEFORMAT (2)}$$

So, $SNR = C(1 - e^{-\beta l})\sqrt{\frac{\rho l}{wt}}$, has a maximum value at thickness $t = 1.26/\beta$, where $\eta = 71.6\%$. And together with Eq. \textbackslash* MERGEFORMAT (2), the maximum SNR for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ can be written as

$$SNR = C' \times 0.638 \sqrt{\frac{\beta}{en_i(\mu_e + \mu_h)}}, \quad \text{\textbackslash* MERGEFORMAT (3)}$$

with $C' = C\sqrt{l/w}$. The intrinsic carrier density n_i is,

$$n_i = 2 \left(\frac{k_B T m_{3D}}{2\pi \hbar^2} \right)^{3/2} e^{-\frac{E_g}{2k_B T}}, \quad \text{\textbackslash* MERGEFORMAT (4)}$$

Where E_g is the band gap, $m_{3D} = \sqrt{m_e m_p}$, and $m_p = (m_{hl}^{3/2} + m_{hh}^{3/2})^{2/3}$, with m_e , m_{hl} , m_{hh} the effective masses for electron, light and heavy holes, respectively. And the mobilities for electrons and holes can be obtained if we assume that all carriers have the same transport relaxation time τ . So

$$\mu_e = \frac{e\tau}{m_e}, \quad \backslash * \text{MERGEFORMAT (5)}$$

$$\mu_h = \frac{n_{hl}}{n_i} \mu_{hl} + \frac{n_{hh}}{n_i} \mu_{hh} = \left(\frac{m_{hl}}{m_p} \right)^{3/2} \frac{e\tau}{m_{hl}} + \left(\frac{m_{hh}}{m_p} \right)^{3/2} \frac{e\tau}{m_{hh}}. \backslash *$$

MERGEFORMAT (6)

What's more, the absorption coefficient β is proportional to the 3D joint density of states $g_{3D} \propto \sqrt{E_{ph} - E_g}$ owing to the Fermi's golden rules. Thus, from Eq. \backslash * MERGEFORMAT (3) and \backslash * MERGEFORMAT (4), we know that

$$SNR \propto \sqrt{\beta/n_i} \propto \sqrt{(E_{ph} - E_g)^{1/2} e^{\frac{E_g}{2k_B T}}} \backslash * \text{MERGEFORMAT (7)}$$

It has a maximum value at $E_g = E_{ph} - k_B T$. For $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$, we can also determine the relation between the band gap E_g and its stoichiometric x through²

$$x = \frac{E_g + 0.3\text{eV} - 5 \times 10^{-4} T}{1.91 - 10^{-3} T}, \quad \backslash * \text{MERGEFORMAT (8)}$$

Therefore, we can obtain m_e , m_{hl} , and m_{hh}

$$m_{hl} \approx m_e = m_0 \left(1 + \frac{2}{3} \left| \frac{E_p}{E_g} \right| \right)^{-1}, \quad \backslash * \text{MERGEFORMAT (9)}$$

$$m_{hh} = 0.4m_0, \quad \backslash * \text{MERGEFORMAT (10)}$$

Where $E_p = (18 + 3x)eV$ with certain x , and m_0 is the free electron mass. We adopt absorption coefficient $\beta \approx 100cm^{-1}$ for $Hg_{1-x}Cd_xTe$ photodetectors¹ in our calculation. Then the maximum SNR for $Hg_{1-x}Cd_xTe$ can be represented only as a function of the photon energy E_{ph} despite the material independent parameter C' .

For TI film, the quantum efficiency $\eta = P$, the dimensionless absorbance we have calculated in the main text. And $R = \rho l/w$, here ρ is the two dimensional surface resistivity. Then we have the SNR for TI film

$$SNR = \frac{I_{ph}}{\sigma_{I_n}} = \frac{2e\eta pS/E_{ph}}{\sqrt{4k_B T \Delta f / R}} = C'P\sqrt{\rho} = C'P\sqrt{\frac{1}{en_i(\mu_e + \mu_h)}}. \quad \text{\textbackslash*}$$

MERGEFORMAT (11)

Next, we need to determine n_i , μ_e , and μ_h for TI thick film and thin films less than 6 quintuple layers (QLs), respectively. For TI thick film, we consider hexagonal warping term in its Hamiltonian $\hat{H} = \hbar v_F (\sigma_x k_y - \sigma_y k_x) + \frac{\lambda}{2} (k_+^3 + k_-^3) \sigma_z$. However, because λ has little effect on m^* , we can still use the effective mass

$m^* \approx \frac{k_B T \hbar^2}{(\hbar v_F)^2}$ without warping term when calculating mobility. So

$$\mu_e = \mu_h = \frac{e\tau}{m^*}. \quad \text{\textbackslash* MERGEFORMAT (12)}$$

As for the carrier density, we numerically obtain it from the TI film's density of states

$$g_{TI}(\varepsilon) = \int d\mathbf{k} \delta(\varepsilon - E(\mathbf{k})),$$

$$n_i = \int_0^{\varepsilon_{cut}} d\varepsilon g_{TI}(\varepsilon) f(\varepsilon, T), \quad \text{\textbackslash* MERGEFORMAT (13)}$$

where $f(\varepsilon, T) = \frac{1}{1 + e^{\varepsilon/k_B T}}$ is the Fermi-Dirac distribution function. Now with Eq. \textbackslash*

MERGEFORMAT (11)~* MERGEFORMAT (13), we can also have the SNR for TI thick film only as a function of the photon energy E_{ph} despite parameter C' .

For TI thin films less than 6 QLs, our rough numerical calculation shows little effect of warping term λ on both its effective mass and carrier density. For the sake of simplicity, we neglect λ when calculating mobility and carrier density. Thus, the

density of state for TI thin film can simply written as $g_{TI'}(\varepsilon) = \frac{m_{thin}^*}{2\pi\hbar^2}$ with the

effective mass $m_{thin}^* \approx \frac{k_B T \hbar^2}{(\hbar v_F)^2}$, and

$$\mu_e = \mu_h = \frac{e\tau}{m_{thin}^*}, \quad \text{* MERGEFORMAT (14)}$$

$$n_i = \frac{k_B T m_{thin}^*}{2\pi\hbar^2} e^{-\frac{E_g}{2k_B T}}. \quad \text{* MERGEFORMAT (15)}$$

This SNR has a maximum value near $E_{ph} = E_g = \Delta$. Again, we have all the material dependent parameters as a function of the photon energy E_{ph} , and the maximum SNR for TI thin film. The parameters for 2~5 QL TI thin films used in calculation are $\Delta=0.252, 0.138, 0.070, 0.041\text{eV}$, $V_a=0, 0.038, 0.053, 0.057\text{eV}$ and $\hbar v_F=3.10, 3.17, 2.95, 2.98\text{eV}\cdot\text{\AA}$,³ respectively.

Finally, because parameter C' is material independent and the same for the $SNRs$ for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and TI films, it is enough for us to calculate the ratio of SNR for TI films over the maximum SNR for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ photodetectors. And the results

$\frac{SNR_{(TI\ thick\ film)}}{SNR_{(Hg_xCd_{1-x}Te)}}$ and $\frac{SNR_{(TI\ thin\ film)}}{SNR_{(Hg_xCd_{1-x}Te)}}$ as a function of the photon energy E_{ph} are plotted in

Fig. 4 in the main text.

References

1. X. Zhang, J. Wang and S. C. Zhang, *Phys. Rev. B*, 2010, **82**, 245107.
2. J. D. Wiley and R. N. Dexter, *Phys. Rev.*, 1969, **181**, 1181.
3. Y. Zhang, K. He, C. Z. Chang, C. L. Song, L. L. Wang, X. Chen, J. F. Jia, Z. Fang, X. Dai, W. Y. Shan, S. Q. Shen, Q. Niu, X. L. Qi, S. C. Zhang, X. C. Ma and Q. K. Xue, *Nat. Phys.*, 2010, **6**, 584.