Hybridization three subbands at Dirac point in special designed strained HgTe thin films with structural inversion asymmetry

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Abstract
We study specially designed strained thin HgTe layers with structural inversion asymmetry (SIA) which allow us to distinguish the topological surface states (TSS) typical for a two dimensional (2D) quantum well system in a subband state. To obtain such a dispersion relation on the basis of the eight-band kp model, the theoretical investigation calculations of thin (below 25 nm wide) HgTe strained films with SIA are investigated. The numerical band-gap engineering and dispersion relation allow us to obtain a new class of materials that are characterized by a Dirac-like dispersion and hybridization of the three different charges describing two TSS and one quantum well subband at $\Gamma$-point (zero gap). This opens up many possibilities from the applications point of view. An external electric field removed this degeneration and opened a band gap between $\Gamma_6$, $\Gamma_{lh}^8$ (lh—light hole) and $\Gamma_{hh}^8$ (hh—heavy hole) subbands characteristic for TSS and the subband characteristic for the 2D quantum well state, respectively. The width of the band gap as a function of the external electric field is also considered. Due to consideration being given to the possible applications, analysis of the dispersion relation and Landau levels (LL) energy shape with SIA is also investigated. The possibility of tuning a band gap is promising from the point of view of, for example, THz detectors and emitters. What is very important, the proposed structures allow the avoidance of the coexistence of TSS with bulk states, as very often occurs in so-called 3D strained HgTe-like materials. Analysis of the wave function as a function of the width of the investigated structure as well as the external electric field is also presented. Due to the strong correlation between both states (2D and TSS), and their very well known properties, we expect that such HgTe films can be used as optical active layers in the THz region.

1. Introduction

So far, many papers have been devoted to HgTe-based systems for which the theoretical and experimental investigation clearly shows that such systems can be treated as typical topological insulators. For HgTe materials two kinds of surface states were experimentally verified: for single quantum wells (QW) with about 6.4 nm wide HgTe [1] and for 3D strained HgTe 75 nm wide films [2–4]. In QWs, e.g. with HgTe 6.4 nm wide, the width of the QW is responsible for the appearance of topological surface states (TSS) at the interfaces. In more complex QWs such as HgCdTe or HgMnTe [6, 7] besides the size, also the chemical composition (in the case of x-Cd and x-Mn compounds) causes TSS that exist at the interfaces between QW and the quantum barrier. On the other hand, for 3D layers uniaxial tensile strain along (001) direction and the proper width of the strained layers are enough to obtain a Dirac cone inside the gap between $\Gamma_6$ and $\Gamma_{lh}^8$ [2]. However, in this case TSS can be observed against the background of the bulk states. Only in a small energy area between the bottom of $\Gamma_6$ and the top of $\Gamma_8$ can pure TSS be observed experimentally [1, 8, 10]. The key question for all of these cases is whether it is possible to obtain such a dispersion relation for which the greatest possible part of the Dirac cone can be seen in the gap between $\Gamma_{lh}^8$ and $\Gamma_{hh}^8$. Recently,
even in a partially relaxed 3D system, TSS have been observed experimentally [9]. But in this case detailed analysis of Shubnikov–de Haas oscillations in both conductivity and capacitance allows three groups of electrons to be distinguished, identified as electrons on top and bottom surfaces and bulk electrons [9].

Many authors are working on more complex systems for which besides the surface states at the interfaces/surface others including, for example, bulk states can be identified [10, 11]. All such investigation is mainly influenced by the very well-known properties of the charge at the surface states such as lack of backscattering. More complex systems also involve structures for which the asymmetry can open an insulating gap by breaking the cubic symmetry at the $\Gamma$ point [12–14]. The coexistence of two different kinds of charge at different electronic levels, for example, for two different surfaces and bulk states, is now one of the most interesting phenomena that allow us to speculate about the application possibilities of such complex systems [7].

The design of the investigated structures in this paper connects properties from both systems: the TSS at the interfaces (characteristic for 3D strained HgTe layers) with the 2D subband states characteristic for 2D electron gas in quantum systems.

From this point of view, we designed 2D strained HgTe thin films with an SIA for which it would be possible to observe the quantum states well defined for two dimensional electron gas in the finite size of QWs, as well as the TSS typical for the HgTe 3D strained systems. Both of them can be found in a small area below 20 nm wide, typical for QW using uniaxial tensile strain, together with SIA typical for 3D systems [2, 8, 15]. The width of the thin HgTe layers is defined in a way to obtain the Dirac point where electronic subbands characteristic for two different surfaces and for QW states meet at the $\Gamma$-point ($k = 0$).

We suggest using specially designed thin films of HgTe situated on the CdTe buffer for which the SIA is defined by the two different environments for both top and bottom surfaces (see inset figures 1(a) and (d)). Never before has the hybridization of three groups of subbands been observed or predicted in such thin strained layers. In this case such a situation takes place. It is similar to that observed for a 3D HgTe 75 nm wide strained system or partly relaxed 200 nm wide HgTe layers. However, the coexisting electrons belonging to the surfaces with electrons characteristic for a QW were not investigated. The advantage of such situations lies mainly in the characteristics of the transport and properties of electrons in quantum states for TSS and QW. The ballistic transport in good quality QWs together with lack of backscattering characteristic for TSS opens up many possible applications in, for example, transport or optical properties.

Our investigation presented here also shows that this hybridization can be removed and tuned by an external electric field, which is very important from the point of view of application possibilities. Our investigation shows that the opened gap is over the maximum of the so-called ‘camel back’ created by the heavy hole subband. This implies that there is no other charge besides the one characteristic for QWs and TSS. The peculiar band structure of HgTe quantum films also gives rise to a unique LL shape. Due to the finite thickness of the investigated structures and the mixture of Landau levels (LL), it is predicted that one of the surfaces at the thin film with the 2D quantum states will be observed.
Our results, presented below, clearly show that the designed material should be verified experimentally due to its special properties and possible applications in the Thz area. This raises many possibilities for the applications of the investigated structures which allow the use of the obtained electron states appearing in thin layers characteristic for surface states and QW state as an active channel for energy transfer with no interference from the bulk current carriers, which is always present in 3D strained HgTe materials. The charge carrying properties of such a system are completely different in comparison to the known semiconductor structures used until today. The sharp interfaces in that case have a large application potential, e.g. for work with terahertz detectors in a magnetic field below 2 T. Our previous work, e.g. [7, 12, 16] shows that SIA has a huge influence on the electronic structures obtained for different kinds of structures (2D as well as 3D strained systems).

2. Theory

In this work the eight-band kp model is used for the calculation of the dispersion relation for the investigated HgTe films in different external conditions. A detailed description of this model, as well as the band parameters used in the calculations and the appropriate exchange term, can be found in [17, 18]. A detailed description of the numerical calculations presented here was obtained by means of the methods elaborated in [19] (Table 1).

The effects of the strain tensor was incorporated in the Kane model through the Bir–Pikus Hamiltonian [20], which can be easily obtained from the Kane Hamiltonian with the substitution $k_lk_j \rightarrow \epsilon_{ij}$ and adopted for the investigated structures. The strain tensor components for the arbitrary growth direction can be determined using the model of De Caro et al [21]. The SIA matrix shape was taken from [22], but there are several potential sources of SIA, e.g. the asymmetric doping profiles, the different alloy compositions of the confining material on either side of the investigated material, the stress fields, the space charge in the layers or the external electric fields in the direction perpendicular to the layers [7]. In this paper external electric magnetic fields were also applied to the thin HgTe films. The Hamiltonian elements for the magnetic field in [19] are presented (e.g. No. 10).

$$ (H_0 + H_{BF} + H_{SLA} + H_{BLA} + H_{SIA} + V(z)) \Psi(z) = E \Psi(z) \quad (1) $$

$$ H_0 = \begin{bmatrix}
T & 0 & -\frac{1}{\sqrt{2}} P k_+ & \frac{1}{\sqrt{2}} P k_z & 0 & -\frac{1}{\sqrt{3}} P k_+ & -\frac{1}{\sqrt{3}} P k_z \\
0 & T & 0 & \frac{1}{\sqrt{6}} P k_+ & \frac{1}{\sqrt{3}} P k_z & 0 & -\frac{1}{\sqrt{3}} P k_+ \\
-\frac{1}{\sqrt{2}} k_P & 0 & U + V & -S_+ & U - V & C & R \\
\frac{1}{\sqrt{2}} k_P & 0 & -S_+ & U - V & C & R & \sqrt{2} V \\
\frac{1}{\sqrt{6}} k_P & \frac{1}{\sqrt{2}} k_P & R^i & C & U - V & \sqrt{2} V & -\sqrt{3} S_+ \\
0 & \frac{1}{\sqrt{2}} k_P & 0 & R^i & \sqrt{2} V & -\sqrt{2} R & \sqrt{2} S_+ \\
-\frac{1}{\sqrt{3}} k_P & -\frac{1}{\sqrt{2}} k_P & \frac{1}{\sqrt{2}} S_+ & \sqrt{2} V & -\sqrt{3} S_+ & \sqrt{2} R & U - \triangle \\
-\frac{1}{\sqrt{3}} k_P & -\frac{1}{\sqrt{2}} k_P & -\sqrt{2} R^i & -\sqrt{2} S_+ & \sqrt{2} R & U - \triangle & C \\
\end{bmatrix} \quad (2) $$

where

$$ k_\parallel^2 = k_x^2 + k_y^2, \quad k_\perp = k_z \pm i k_y, \quad k_z = -i \partial / \partial z \quad (3) $$

$$ T = E_c(z) + \frac{\hbar^2}{2m_0} [(2F + 1) k_\parallel^2 + k_z (2F + 1) k_z], \quad (4) $$

$$ U = E_c(z) - \frac{\hbar^2}{2m_0} (\gamma_1 k_\parallel^2 + k_z \gamma_1 k_z), \quad (5) $$

$$ V = -\frac{\hbar^2}{2m_0} (\gamma_2 k_\parallel^2 - 2 k_z \gamma_2 k_z), \quad (6) $$

$$ R = -\frac{\hbar^2}{2m_0} \sqrt{3} (\mu k_\parallel^2 - \gamma_3 k_z^2), \quad (7) $$

3
As mentioned before, the asymmetry and its influence on the shape of the TSS are the most widely discussed subjects in the case of HgTe materials [23]. It is worth mentioning that the symmetric (013) oriented QW based on HgTe with critical and close-to-critical thickness was considered from the point of view of the influence of interface inversion asymmetry (IIA) at heterojunctions [24]. The authors claim, however, that IIA defined in this way removes only the spin degeneracy but leaves a valley degeneracy and is unstable. This effect also depends on, inter alia, the fact that the walls of the QWs are grown under different conditions. This means that the influence of this effect is much weaker than that caused by asymmetric structures with strong SIA. This effect depends on many factors, is unstable and may not be intentional [25]. In our calculation we use (001) oriented HgTe films and due to the small influence of the IIA and its unintentional and incidental influence that comes directly from the methods of MBE growth promotion, this effect was omitted in our investigation.

3. Results

Applying a uniaxial tensile strain to a HgTe QW with Dirac-like dispersion can be observed for approx. 7.1 nm wide HgTe QW. Such a situation is presented in figure 1(a) (for 7.1 nm wide HgTe films) and 1(d) (for 12.3 nm wide HgTe films), while the dispersion relation and LLs structure are presented respectively—figure 1(b) (LLs for 7.1 nm HgTe) and 1(c) (LLs for 12.3 nm HgTe). So in the very well known critical thickness for 6.4-wide HgTe QW the difference is a few monolayers. For 12.3 nm wide HgTe films the 1 nm CdTe cap was defined on the up surface (see figure 4). It is enough to fulfill the SIA effect.

At Γ point (k = 0) three different subband types meet for 12.3 nm wide strained HgTe films. At this point the shapes of the wave vectors of the TSS are presented in figure 2(d). This is a unique and important situation, while the hybridization of Γ6, Γ8h, Γ6b were expected. Such a case has not so far been observed in experimental results or in theoretical predictions. It raises many possibilities from the application point of view. From this point of view, the possibility of the opening of this gap by the external electric field was also investigated—see figure 2(a). The external electric field can open this gap and for U = 0.12 V this gap is about 11 meV. The dispersion relation for this case is presented in the inset of figure 2(a)—right bottom corner scheme. This case is very promising due to the fact that the obtained gap is not covered by the top of the 5th band for k > 0. In the opposite case, for U = −0.12 V the induced gap is entirely covered by the heavy hole subband see inset of figure 2(a)—upper left corner.

In figure 2(b) the shape of the wave functions for four values of energy and its dependents along the z direction is presented for an external electric field equal to 0. It is clearly visible that along the z direction the wave functions characteristic for TSS for a surface with 1 nm CdTe cap layer overwhelm the TSS characteristic for the second surface (from the bottom side). Together with the increasing k-vector the wave functions have a mixed character (see the blue curves for k about 0.04 nm⁻¹). To show what the energy dispersion looks like as a function of the temperature, the necessary calculations were also carried out for 200 K, and the results are presented in figure 2(c). For the strained symmetric HgTe films (open box) the zero gap can be obtained in the temperature region from 4.2 K up to 200 K. For 200 K the width of the HgTe films is about 5.2 nm for which the energy gap is 0. In the case of an asymmetric structure for 200 K

| HgTe | CdTe | HgTe | CdTe |
|------|------|------|------|
| E₀   | 0.303 eV | 1.606 eV | C | −3.83 eV | −4.06 eV |
| E₁   | 0 | −570 meV | a | 0 | −0.7 eV |
| Δ    | 1.08 eV | 0.91 eV | b | −1.5 eV | −1.17 eV |
| E₂   | 18.8 eV | 18.8 eV | d | −2.08 eV | −3.2 eV |
| F    | 0 | −0.09 | C₁ | 53.6 GPa | 53.6 GPa |
| γ₁   | 4.1 | 1.47 | C₁ | 36.6 GPa | 37.0 GPa |
| γ₂   | 0.5 | −0.28 | C₁ | 21.2 GPa | 19.9 GPa |
| γ₃   | 1.3 | 0.03 |
| κ    | −0.4 | −1.31 |

γ₃ = \frac{\hbar^2}{2m_0} \sqrt{3k_z (\gamma_3, k_z + \{\kappa, k_z\})},

Sₚ = \frac{\hbar^2}{2m_0} \sqrt{3k_z \left( \gamma_3, k_z \left\{ -\frac{1}{3} (\kappa, k_z) \right\} \right)},

C = \frac{\hbar^2 k_{\pm}}{m_0} (\gamma_3, k_z).
there is no zero gap energy up to 20 nm wide. Our approximation shows that even for 35 nm it is not possible to obtain a zero gap. After this width the properties of so-called 3D strained systems appeared. For 4.2 K the gap is zero for 12.3 nm width of strained HgTe films, after that it opens again to reach zero in approximation to strained 3D HgTe layers [5].

An external electric field can open an energy gap between $\Gamma_{hh}$ and $\Gamma_{lh}$ as was presented in figure 2(a). To see the nature of the correlations between the TSS and the quasi 2D subband states, the distribution of the wave functions according to the separation of the charge channel between these two physically different states were also calculated. In figure 4 such results are presented for two different external electric fields: $U = -0.12$ V (figures 4(a)–(d)) and $U = 0.12$ V (figures 4(e)–(h)). An external voltage equal $-0.12$ V caused that a TSS characteristic for the bottom surface is visible. At the same time, the maximum
Figure 4. The scheme of the experimental setup to measure the kinds of current: one characteristic for TSS and one characteristic for a quasi-2D quantum state.

probability of the heavy hole charges is moved in this direction. For $U = 0.12$ V a wave function characteristic for TSS of the up surface is much more visible. However the maximum of $|\Psi_{hh}|^2$ is very close to the up surface. All these calculations were carried out for $k = 0$. In figure 2(d) the distance between $|\Psi_{hh}|^2$ and $|\Psi_{TSS}|^2$ is plotted versus the external electric field. Such analysis shows that using the designed system it is possible to show and investigate the nature of correlated Dirac fermions in such a unique system as the one investigated in this paper with a quasi 2D band. With no so-called bulk conductivity, as is always present in 3D strained HgTe films, the TSS in our systems can be verified in much more detail.

4. Conclusion

We have studied specially designed strained thin HgTe layers with structural inversion asymmetry (SIA) under an external electric and magnetic field from the point of view of the shape of the dispersion relation (see figure 4). The obtained results allow us to conclude that for such special HgTe strained layers of width about 12.3 nm the $e\Gamma_6$-points have triple degeneracy and three different energy states: two characteristic for surface states ($\Gamma_6$ and $\Gamma_{lh}$) and one characteristic for a QW subband ($\Gamma_{hh}$). The design of the investigated structures in this papers connects properties from two systems: the TSS at the interfaces (characteristic for 3D strained HgTe layers) with the 2D subband states characteristic for 2D electron gas in quantum systems. This is a unique and important situation that has never been investigated before, which opens up new possibilities. The mixed states characteristic for three states, or in principle two (one overwhelming surface state and one 2D quantum state), together with the possibility of tuning the energy gap allow us to think about applications possibilities.

Having in mind the numerical calculations presented in this paper together with the diagram of the designed structures (figure 4) it is obvious that such structures in designed configuration can serve as an excellent example for experimental investigation of the correlation between TSS and 2D subbands—figure 4. Applying an external electric field together with the possibility of measuring the two kinds of current: one characteristic for TSS and one characteristic for a quasi-2D quantum state, can give information about complex systems as well as separated energy transfer along the investigated 12.3 nm wide HgTe films. Experimental observation of the mixture of the LLs belonging to surface states and 2D quantum systems would be an important advancement in understanding the nature of correlated Dirac fermions in such a unique system as the one investigated in this paper. The proposed experiment should be carried out following the method presented in [8].

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.
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