Solid State Communications 251 (2017) 1–4

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Communication

Electric field dependence of hybridized gap in InAs/GaSb quantum well system

Jiufu Ruan[a], Xiangfei Wei[b,*], Weiyang Wang[c]

[a] Academy of Photoelectric Technology, Hefei University of Technology, Hefei 230009, China
[b] College of Materials and Chemical Engineering, West Anhui University, Luan 237012, China
[c] School of Physics and Electronics Information,Shangrao Normal University, Shangrao, Jiangxi 334001, China

ARTICLE INFO

Keywords:
External electric field
Type II and broken-gap quantum well
Exchange self-energy
Hybridized gap

ABSTRACT

We demonstrate theoretically that exchange interaction induced by electron-hole scattering via Coulomb interaction can cause a hybridized gap in InAs/GaSb based type II and broken-gap quantum wells. The hybridized energy spectra are obtained analytically at the low temperature and long wave limits. An electric field depended hybridized gap about 4 meV opens at the anti-crossing points of the hybridized energy spectra, in accordance with experimental measurements. The hybridized gap varies linearly with the gate electric voltage due to the fact that the electric field can change the exchange self-energy by tuning the overlap of the wavefunctions and the Fermi energy. Our theoretical results can give a deep insight of the origin of the hybridized gap and provide a simple way to determine the value and the position of the hybridized gap in the presence of the gate electric voltage.

1. Introduction

The properties of the InAs/GaSb quantum well system (QWs) have been investigated intensively ever since it was proposed in 1983 [1] for its broken-gap band alinement at the interface. A type II and broken-gap quantum well system (T2BGQWs) can be formed with a wide width of the InAs layer and a narrow width of the GaSb layer, in which the hole subband energy can be higher than the electron subband energy. The InAs/GaSb based T2BGQWs has been considered to be one of the most promising systems for the fundamental physics and the design of photoelectric devices, especially in the third generation of infrared detectors [2,3]. Most recently, the InAs/GaSb based T2BGQWs has shown evidences for the existence of the topological insulators(TI) phase [4–7] due to the opening of a hybridized gap at the anti-crossing points of the hybridized energy spectra. In two-dimensional materials, the TI phase was first predicted to occur in graphene [8] and strained GaAs [9], shortly thereafter in inverted HgTe/CdTe QWs [10] and InAs/GaSb composite QWs [4]. HgTe/CdTe QWs is recognized to be the most ideal material in the investigations of the TI phase. However, the mercury content in HgTe/CdTe QWs imposes some strict fabrication restrictions and in this TI material, the TI phase can be modulated only through changing the thickness of the quantum well. On the other hand, InAs/GaSb based T2BGQWs is another mature material with well developed molecular beam epitaxy growth and device fabrication techniques. Compared to HgTe/CdTe QWs, the InAs/GaSb based QWs has numbers of advantages, including low Schottky barriers to most metals, with good interface to superconductor [11], and most importantly with continuously tunable subband energy via the gate electric voltage, which makes this material uniquely suit for the study of the phase transition from TI to normal insulator via varying the external electric field continuously.

In the InAs/GaSb based T2BGQWs, a hybridized gap can open at the anti-crossing points of the electron and hole energy spectra due to the coupling of electron and hole at the interface. Most importantly intensive theoretical and experimental studies have indicated that Coulomb interaction between electron and hole in different material layers plays a dominant role in opening a gap in InAs/GaSb based T2BGQWs [12–15]. In the experimental investigations of the TI phase, it is one of the necessary conditions to tune the Fermi energy level into the hybridized gap through applying the gate electric voltage or changing the widths of the QWs [4]. In the present study, attentions are paid to the dependence of the hybridized gap on the external electric field. We notice that both the subband energies and the overlap of the wavefunctions can be modulated during tuning the Fermi energy level into the hybridized gap. Therefore, the hybridized gap can be modulated by the external electric voltage. From a viewpoint of fundamental physics and design of novel devices, it is significant and necessary to examine the dependence of the hybridized gap on the gate

* Corresponding author.
E-mail addresses: flyxfwei@sina.com (X. Wei), wywang2014@sina.cn (W. Wang).

http://dx.doi.org/10.1016/j.ssc.2016.12.001
Received 31 August 2016; Received in revised form 16 November 2016; Accepted 1 December 2016
Available online 05 December 2016

electric voltage in InAs/GaSb based T2BGQWs and this has become one of the prime motivations of this theoretical study.

2. Theoretical considerations and approaches

In this study, we take the growth direction of the quantum well along the z-axis. The Schrödinger equation for an electron or a hole in the presence of the gate electric voltage can be written as

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(z) - qFz\right]\psi(z) = E\psi(z), \tag{1}$$

where m^* is the effective mass of the carriers. Here, $V(z)$ is the confining potential energy for an electron or a hole along the growth direction of the quantum well, $q = -e$ for an electron and $q = +e$ for a hole, F is the strength of the external electric field, and $\psi(z)$ is the wavefunction along the growth direction for an electron or a hole.

There is no simple analytical solution to the Schrödinger equation under the external electric field. The transfer matrix approach is employed to solve the Schrödinger equation numerically, which has been proved simple and accurate [16]. As the effect of the self-consistent potential only shifts the band edges of the QWs, which is reasonably neglected in the present calculations. After dividing the QWs into N layers, the wavefunction within the$l$-layer can be expressed as a linear combination of complex exponential functions

$$\psi_l(z) = A_l e^{ik_l z} + B_l e^{-ik_l z}, \tag{2}$$

where $k_l = \sqrt{2m_l^*(E - V_l)}/\hbar$ is a complex function. Considering the continuity conditions for the wavefunction and the particle current, the relationship between the constants A and B in the $(l + 1)$-layer and the l-layer is obtained

$$\begin{bmatrix} A_{l+1} \\ B_{l+1} \end{bmatrix} = M_l \begin{bmatrix} A_l \\ B_l \end{bmatrix}, \tag{3}$$

where M_l is a 2×2 matrix [16]. Consequently the relationship between A and B in the outermost layers can be obtained

$$\begin{bmatrix} A_{N-1} \\ B_{N-1} \end{bmatrix} = M_{N-2}\cdot M_{N-1}\cdot\cdots M_1\cdot M_0 \cdot \begin{bmatrix} A_0 \\ B_0 \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}\cdot\begin{bmatrix} A_0 \\ B_0 \end{bmatrix}. \tag{4}$$

N is the total number of the divided layers. The energy eigenvalue E can be calculated by $M_{22}(E) = 0$, which is derived from the boundary conditions $A_0 = 0$ and $B_{N-1} = 0$.

In InAs/GaSb based T2BGQWs, only the lowest electron subband and the highest hole subband are experimentally relevant, we therefore consider the T=0 K situation with only the lowest electron subband and the highest hole subband occupied. The electrostatic energy induced by the carrier-carrier (c-c) scattering through the Coulomb interaction can be calculated with the single-particle wave functions. In an electron-hole two-particle system, the dielectric function under the random phase approximation (RPA) canbe written as a 2×2 matrix [14,17]

$$\epsilon(\Omega, q) = \begin{bmatrix} 1 - A_{ee} & A_{eh} \\ A_{he} & 1 - A_{hh} \end{bmatrix}, \tag{5}$$

where the Auger recombination and impact ionization are neglected [18]. Here, $A_{jj'}(\Omega, q) = V_q^j \Pi_{jj'}(\Omega, q) F_{jj'}(q)$ with the bare Coulomb interaction in two-dimensional electron gas $V_q^j = 2\pi e^2/(\kappa_j q)$, κ_j is the static dielectric constant, $\mathbf{q}$ is the change of the wavevector, Ω is the excitation energy, $F_{jj'}(q) = \int dz_1 \int dz_2 \, |\psi_0^{j'}(z_1)|^2 |\psi_0^j(z_2)|^2 e^{-q|z_1 - z_2|}$ is the so-called form factor depending on the overlap of the wavefunctions during a scattering event and $\Pi_{j'j}(\Omega, q)$ is the density-density correlation function under RPA [19].

The screened energies for Hartree ($\alpha = H$) and exchange($\alpha = E$) interactions are calculated through $U_{jj'}^{\alpha *} = \epsilon_{jj'}^{-1}(q) U_{jj'}^{\alpha}$, where $U_{jj'}^{\alpha}$ is the Hartree ($\alpha = H$) or exchange ($\alpha = E$) interactions in the absence of the c-c screening and $\epsilon_{jj'}(q) = \lim_{\Omega \to 0} \epsilon_{jj'}(\Omega, q)$ is the element of the static dielectric function matrix [14]. In the present study, the effect of the Hartree interaction is neglected due to the fact that the Hartree self-energy only provides a constant energy background [20]. At the low-temperature limit ($T \to 0$ K), the exchange self-energy is expressed as

$$\Xi_{jj'}(k) = -\sum_{\mathbf{k}' < \mathbf{k}_F^j} \frac{2\pi e^2}{\kappa_j [q + K_{jj'}(q)]} F_{jj'}(q) \delta_{\mathbf{k}', \mathbf{k}+\mathbf{q}}, \tag{6}$$

where $\mathbf{k}_F^j$ is the Fermi wavevector of the carriers. Here, $K_{jj'}(q)$ is the inverse screening length for a scattering event under RPA, which can be obtained analytically at the long wave limit, that is, $K_{jj'} = \lim_{q \to 0} K_{jj'}(q) = \frac{2e^2}{\hbar^2 \kappa_j} \frac{m_e^* m_h^* - M^2}{m_{j'}^* + M}$, with $M = [\ln(m_h^*/m_e^*)] m_e^* m_h^*/(m_e^* + m_h^*)$.

The many-body Green's function for a quasi-particle is obtained fromthe diagrammatic techniques [21], which reads $G_{j'j}(E, k) = [G_j^{-1}(E, k) - \Xi_{j'j}(k)]^{-1}$, with the non interacting Green's function $G_j(E, k) = [E - E_k^j + i\delta]^{-1}$. The quasi-particle energy dispersions are determined by the poles of the Green's function

$$E_{\pm}(k) = \frac{1}{2}[E_k^e + \Xi_{ee}(k) + E_k^h + \Xi_{hh}(k) \pm \sqrt{[E_k^e + \Xi_{ee}(k) - E_k^h - \Xi_{hh}(k)]^2 + \Delta(k)^2}\,], \tag{7}$$

where $\Delta(k) = 2\sqrt{\Xi_{eh}(k)\Xi_{he}(k)}$ is a k-dependent minigap depending on the exchange self-energy $\Xi_{eh}(k)$ and $\Xi_{he}(k)$. It should be noticed that, the hybridized gap evokes from the exchange scattering between electrons and holes. Generally, the hybridized gap $\Delta E(k_F) = |E_+(k_F) - E_-(k_F)|$ at the anti-crossing points of electron and hole energy spectra can be valued with the minigap $\Delta(k_f)$. As can be seen, the minigap $\Delta(k)$ depends on both the Fermi wavevector and the form factor $F_{jj'}(q)$, both of which can be modulated conveniently by theexternal electric filed. Consequently, the hybridized gap can be modulated via the external electric field in InAs/GaSb based T2BGQWs. In this paper, the dependence of the hybridized gap on the gate electric voltage will be illustrated in detail.

3. Numerical results and discussions

In this study, attentions are focused on the dependence of thehybridized gap on the external electric field in InAs/GaSb basedT2BGQWs. The transfer matrix approach is employed to solve theSchrödinger equations under the external electric field to get thesubband energies as well as the wavefunctions both for electron and hole. A set of typical QWs widths $L_{InAs} = 12.5$ nm and $L_{GaSb} = 10$ nm are taken throughout the calculations. We take themass of the electron in the InAs layer as $m_e^* = 0.038 m_e^0$ and themass of the hole in the GaSb layer as $m_h^* = 0.33 m_e^0$, with m_e^0 being the rest mass of an electron. The static dielectric constants in the InAs layer and the GaSb layer are taken as $\kappa_e = 15.15$ and $\kappa_h = 15.69$, respectively. The direction from the InAs layer to the GaSb layer is taken as the positive direction of the electric field. And the reference point of the energy is put at the bottom of the conduction band in the InAslayer.

In InAs/GaSb based T2BGQWs, electrons and holes are separated spatially. The overlap of electron and hole wavefunctions can be tuned with the gate electric voltage. As can be seen in Fig Fig 1(a), the wavefunctions for electron and hole are separated from each other by the positive electric field (e.g. $F = 40$ kV/cm) and combined with the negative electric field (e.g. $F = -40$ kV/cm) due to their different charge. The ground-state subband energies in thepresence of the external electric filed are shown in Fig. 1(b). Thesubband energy for electron increases linearly with the external electric field and the subband energy for hole decreases linearlywith the external electric field due to their different charge [22]. Therefore, both the subband energies and the overlap of the wavefunctions can be significantly affected by the external electric field in InAs/GaSb based T2BGQWs, which will affect the self-energy significantly.

In the calculations of the exchange self-energy, the