Heterostructures, superlattices, quantum wells

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Effects of resonant tunneling in GaAs/AlAs heterostructure

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Abstract. We investigate the effects of resonant tunneling of the charge carriers of the Γ_8 zone in the GaAs/AlAs heterostructure within the framework of the effective mass method, taking into account complex character of the valence band dispersion law. The problem is solved by introducing Green's function with parametric dependence on energy within the biorthogonal formalism of quantum theory. The effects imposed by the spin state of holes, as well as the effect of short-range interface corrections, are investigated.

Keywords: heterostructures, hole tunneling, resonant tunneling

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Материалы конференции
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Эффекты резонансного туннелирования в гетероструктуре GaAs/AlAs

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Аннотация. В работе исследуются эффекты резонансного туннелирования носителей заряда зоны Γ_8 в гетероструктуре GaAs/AlAs в рамках метода эффективной массы с учетом сложного характера закона дисперсии валентной зоны. Задача решается с помощью введения функции Грина с параметрической зависимостью от энергии в рамках биортогонального формализма квантовой теории. Исследованы эффекты, накладываемые спиновым состоянием дырок, а также влиянием короткодействующих интерфейсных поправок.

Ключевые слова: гетероструктуры, туннелирование дырок, резонансное туннелирование

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Introduction

Resonant tunneling in quantum-dimensional structures is the charge carrier transfer through potential barriers of finite height when its energy is equal to the resonance energy of the quantum system. This phenomenon is used in the design of a variety of electronic devices working at high frequency and terahertz range: semiconductor optic amplifiers and modulators, quantum-cascade structures and others [1—5]. Another field of application is spintronics where polarization effects are used to separate charge carriers with various effective spin momentum projections. It makes it possible to design different spintronic devices like spin filters and spin injectors [6, 7].

Theoretically, tunneling processes are described by the transmission coefficient which is equal to the relation of probability flow densities. To find probability flow, we need to solve the stationary inhomogeneous Schrodinger equation. In general case, it has the following operator form

$$\left[\hat{H} - E\right]\left|\psi\left(E\right)\right\rangle = \left|\rho\right\rangle, \tag{1}$$

where $\hat{H}$ is the Hamiltonian of the quantum system, $|\psi\,(E)\rangle$ is vector, which describes the stationary state of the quantum system with energy E and $|\rho\rangle$ is vector characterizing the particle source in the quantum system.

The Schrodinger equation is generally solved by the transfer matrix method. This approach has a high calculation precision, however, it requires large software capacities and is also associated with the need to satisfy a large number of boundary conditions in the case of multi-barrier structures and the complex structure of the energy zones of the materials [8, 9].

In the present work, effects of resonant tunneling in heterostructures are investigated using Green's function method which can be formulated within the framework of the biorthogonal approach to the analysis of quantum systems described by non-Hermitian operators [10, 11]. The problem is reduced to a solution of the inhomogeneous Schrodinger equation in the k-representation using the corresponding Green's function, parametrically dependent on energy. In the case of the open unlimited space, the particle wave function amplitude is not equal to zero at infinity. Accordingly, the system Hamiltonian is non-Hermitian. Within the framework of the developed approach, a finite space is considered and a method of smoothly changing dissipative potential barriers near the boundaries of the structure into the system is applied. In the region of this dissipative potential, the amplitude of the wave function of the particle fades. The presence of a potential of this kind leads to the fact that the Hamiltonian of a particle in a limited region also becomes non-Hermitian. Consequently, the solution of the problem with the escape of a particle to infinity can be replaced by the solution of the problem in a finite-size space with the analogous non-Hermitian Hamiltonian [12].

Theory

The mathematical formulation of the biorthogonal theory is based on the search for two sets of eigenvectors and eigenvalues of a given non-Hermitian Hamiltonian and its conjugate operator. The problems of finding eigenvalues and eigenvectors have the form

$$\begin{aligned} \hat{H}\left|\psi_n^r\right\rangle &= E_n\left|\psi_n^r\right\rangle, \\ \hat{H}^{\dagger}\left|\psi_n^l\right\rangle &= E_n^{\dagger}\left|\psi_n^l\right\rangle, \end{aligned} \tag{2}$$

where $\left|\psi_n^r\right\rangle$ and $\left|\psi_n^l\right\rangle$ are 'right' and 'left' eigenvectors respectively, related by the biorthonormality and completeness conditions

$$\begin{aligned} \left\langle\psi_n^l\middle|\psi_{n'}^r\right\rangle &= \delta_{nn'}, \\ \sum_n\left|\psi_n^r\right\rangle\left\langle\psi_n^l\right| &= 1. \end{aligned} \tag{3}$$

The tunneling problem is considered within the framework of Green's function method, which is convenient for analyzing a continuous energy spectrum. Green's function for the Schrodinger equation, parametrically dependent on the energy of a particle, has the operator form

$$\hat{G}(E)=\left(\hat{H}-E\right)^{-1}. \tag{4}$$

Using the Kohn–Luttinger basis, we can solve the Schrodinger equation (1) within the framework of the effective mass method [13]. The effective Hamiltonian of Γ_8 zone in k-representation has the form

$$H^{(\Gamma_8)}=\frac{\hbar^2}{2m_0}\begin{bmatrix} P+Q & W & V & 0 \\ W^\dagger+ & P-Q & 0 & V \\ V^\dagger & 0 & P-Q & -W \\ 0 & V^\dagger & -W^\dagger & P+Q \end{bmatrix}, \tag{5}$$

where $P=\gamma_1\left(k_x^2+k_y^2+k_z^2\right)$, $Q=\gamma_2\left(k_x^2+k_y^2-2k_z^2\right)$, $V=-\sqrt{3}\gamma_2\left(k_x^2-k_y^2\right)+i2\sqrt{3}\gamma_3 k_x k_y$, $W=-2\sqrt{3}\gamma_3\left(k_x-ik_y\right)k_z$, γ_1, γ_2, γ_3 are Luttinger parameters characterizing structure of the valence band. For a finite volume of the system, wave vector k is taking discrete values.

Thus, we can determine the solution of Eq. (1) with the Γ_8 effective Hamiltonian using the corresponding Green's function

$$\langle k|\psi(E)\rangle=\sum_{k'}\langle k|\hat{G}(E)|k'\rangle\langle k'|\rho\rangle. \tag{6}$$

Results and Discussion

In this work, tunneling of holes in a one-dimensional double barrier heterostructure GaAs/AlAs is investigated. The system has the following parameters: width of quantum well d_w = 20 nm, width of quantum barriers d_b = 30 nm, the energy gap between two materials is 0.46 eV. The k_y and k_z components of wavevector k are equal to zero. Luttinger parameters for GaAs: γ_1 = 6.98, γ_2 = 2.06, γ_3 = 2.93. Luttinger parameters for AlAs: γ_1 = 3.76, γ_2 = 0.82, γ_3 = 1.42 [14]. The characteristic functions of the potentials and energy dependence of the tunneling coefficient are shown in Figs. 1 and 2, respectively.

Quantum barriers are formed by AlAs atoms and quantum well potential is formed by GaAs atoms. The dissipative potentials at the boundaries of the region are located at some distance from the quantum barriers and are set smoothly enough so that their effect on tunneling is excluded. Source of particles is set on the left side in front of the first barrier.

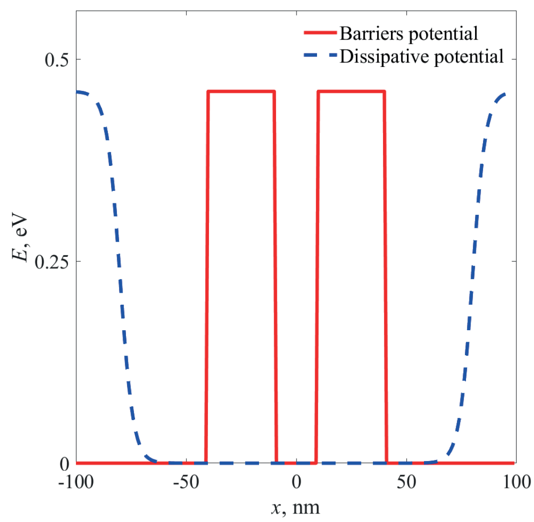

Fig. 1. Double barrier structure (red solid line) with dissipative potential (blue dotted line) near the boundaries

As shown in Fig. 2, the energy dependence of transmission coefficient has several resonant peaks. The first of them are low-intensity resonant peaks located before the energy of the quantum barrier. They correspond to the tunneling of holes with energy below the height of the barrier. It is possible due to the existence of quasi-resonant energy levels in quantum well between two barriers. The last peak in this energy range is located after the energy of quantum barriers and corresponds to the transition of holes with energy higher than the height of quantum barriers. The width of these peaks is related to the lifetime of charge carriers in the quantum system – a smaller width corresponds to a longer lifetime of charge carriers.

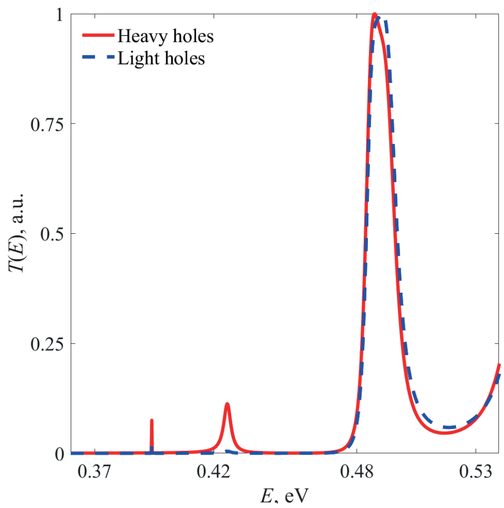

Fig. 2. Tunneling ration depending on the energyfor heavy (solid red line) and light (dashed blue line) holes

Let us consider the structure with non-zero k_y and k_z components of wavevector **k**. Energy dependence of the transmission coefficient in such system is shown in Fig. 3.

In this case, energy dependence of the transmission coefficient is different for holes with all spin projections. The shift of the second series of resonant peaks is approximately 20 meV. As illustrated in Fig. 3, holes with different spin projections have their own resonant energies: at the first resonant peak heavy holes with both spin projections are tunneling with the same probability and with the same energy. However, light holes have different tunneling probabilities and resonant energies. At the next resonant peak, there is increasing intensity of the second resonant peak. The shift of this series is too small.

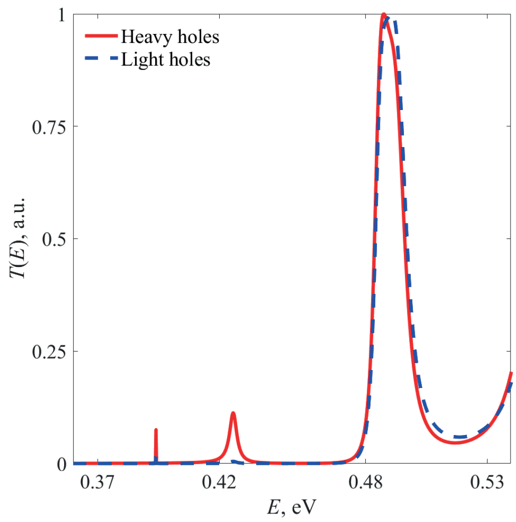

Fig. 3. Tunneling ratio depending on the energy for holes with different effective spin projections (m_S = +3/2 is marked by the solid red line, m_S = +1/2 by the solid blue line, m_S = –1/2 by the dashed blue line, m_S = –3/2 by the dashed red line)

Since the heterostructure consists of two different materials, we need to consider the influence on resonant tunneling from both of them. GaAs and AlAs have different dispersion laws, so we need to include in our model the changing of Luttinger parameters and thus take into account the effect of the interface on the holes with a certain spin projection: $\gamma^i_{\mathbf{kk}'} = \gamma^i \delta_{\mathbf{kk}'} + \Delta\gamma^i f_{\mathbf{kk}'}$, where $\Delta\gamma^i = \gamma^i_1 - \gamma^i_2$. Tunneling coefficient dependent on energy for heavy holes with spin projection +3/2 is shown in Fig. 4. The k_y and k_z components of wavevector $\mathbf{k}$ are equal to zero.

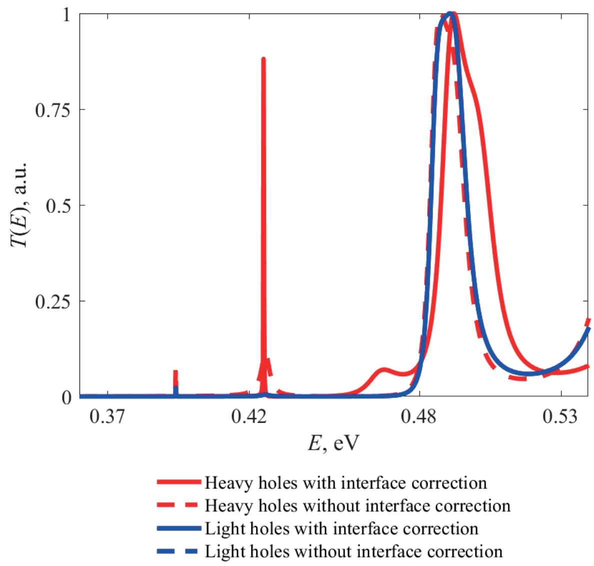

Fig. 4. Difference between tunneling ratio depending on the energy for two cases (the case with interface correction corresponds to the solid red line, the case without interface correction to the dashed blue line)

We can observe increasing intensity of the first resonant peaks and shift of the second series of peaks. The shift is approximately 15 meV. There are two different peaks for independent tunneling of heavy holes and light holes because these interface corrections including change of Luttinger parameters do not influence light hole tunneling.

Finally, we investigate the Rashba effect of the interaction of a heavy hole with effective spin projection +3/2 and the interface of the quantum structure. To introduce these corrections, we need to use the effective Hamiltonian. Its kinetic energy is the sum of Hamiltonian (5) and Rashba Hamiltonian (6). The dependences of the tunneling coefficient are compared in Fig. 5 taking into account the Rashba effect and without it.

$$\Delta H^{(\Gamma_8)} = i\frac{\hbar^2}{2m_0}\Delta R\begin{bmatrix} R_1 & R_3^\dagger & 0 & 0 \\ R_3 & R_2 & R_4^\dagger & 0 \\ 0 & R_4 & -R_2 & R_3^\dagger \\ 0 & 0 & R_3 & -R_1 \end{bmatrix}, \qquad (6)$$

where $R_1 = \frac{3}{2}\left(k_x k'_y - k_y k'_x\right)$, $R_2 = \frac{1}{2}\left(k_x k'_y - k_y k'_x\right)$, $R_3 = \frac{\sqrt{3}}{2}\left[\left(k_y k'_z - k_z k'_y\right) + i\left(k_z k'_x - k_x k'_z\right)\right]$, $R_4 = 2\left[\left(k_y k'_z - k_z k'_y\right) + i\left(k_z k'_x - k_x k'_z\right)\right]$, ΔR is interface correction amplitude.

It can be seen from Fig. 5 that there is the shift of resonant peaks for heavy holes with spin projection +3/2 with energy more than the height of the quantum barrier. It is approximately 20 meV. Additionally, there is another shift of the peak in the low-energy range, which is approximately 10 meV.

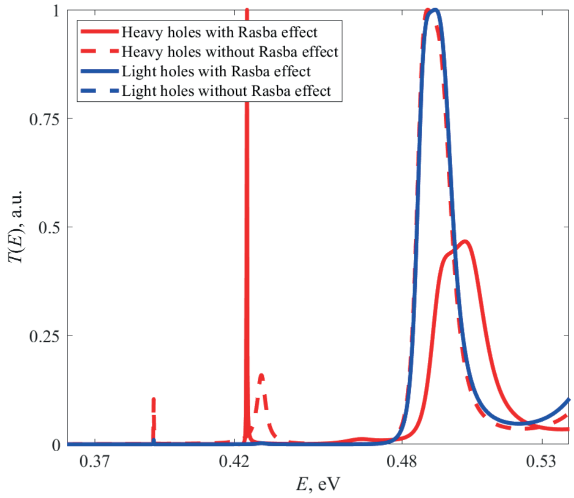

Fig.5. Difference between tunneling ratio depending on the energy for two cases (solid red line corresponds to the case with the Rashba effect, dashed blue line to the case without the Rashba effect)

Conclusion

The effects of resonant tunneling of charge carriers in a GaAs/AlAs heterostructure with a system of two potential barriers are investigated. The tunneling of holes in the Γ_8 zone is considered, where a significant role is played by the difference in the dispersion of particles corresponding to different spin projections. The influence of short-range interface corrections related to the difference in the dispersion law in the materials forming the heterostructure is also considered. In particular, the change in the transmission coefficient is shown when taking into account the interface effect of Rashba. Shifts of tunneling ratio resonant peaks are shown and estimated. The investigated heterostructure can be used to design spintronics devices.

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