Resonance transparency of an abrupt heterojunction

M. V. Kisin and V. I. Petrosyan
Institute of Radio Engineering and Electronics, Saratov Branch of the Academy of Sciences of the USSR

(Submitted 15 June 1989)
Pis'ma Zh. Eksp. Teor. Fiz. **50**, No. 2, 84–86 (25 July 1989)

A resonance (reflectionless) transmission of a conduction electron through an abrupt heterojunction situated between two semiconductors, of which the narrow-band semiconductor has the lesser electron affinity, is predicted.

The presence of an abrupt interface between two wave-carrying media generally leads to a partial reflection of the incident wave. In the conduction band of an abrupt heterojunction this process corresponds to a quantum-mechanical effect of the above-the-barrier reflection.[1] As a result, the transmission coefficient T, which is equal to the

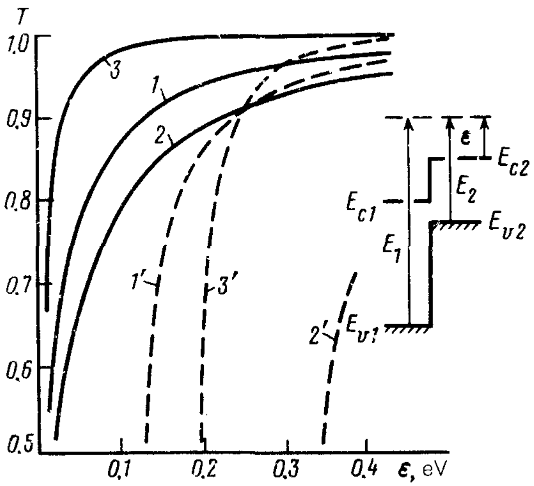

FIG. 1. Transmission coefficient of various heterojunctions. 1, 1'—GaAs-GaAlAs, $E_{g1}\sim 1.4$, $E_{g2}\sim 2.0$, $\Delta_1\sim\Delta_2\sim 0.3$, $\Delta_v\sim 0.2$ eV; 2,2'—InAs-GaSb, $E_{g1}\sim\Delta_1\sim 0.4$, $E_{g2}\sim\Delta_2\sim 0.8$, $\Delta_v\sim 0.5$ eV; 3,3'—InAs-InSb, $E_{g2}\sim 0.2$, $\Delta_2\sim 0.9$, $\Delta_v\sim 0.5$ eV (Ref. 6). Curves 1–3 correspond to $K=0$. The inset shows the relative arrangement of the bands, which accounts for the resonance.

ratio of the fluxes of the transmitted and incident waves, must be less than unity. A resonance transition ($T=1$) can occur in the presence of two interfaces if there is an appropriate interference in the region between them.[2] We will show, however, that at $\Delta_c\equiv E_{c2}-E_{c1}>0$, $\Delta_v\equiv E_{v2}-E_{v1}>0$, and $E_{g1}>E_{g2}$ (see Fig. 1) a conduction electron can undergo a reflectionless resonance transmission through a single interface.

It is clear that such an effect is closely related to the specified boundary conditions. The wave-function-envelope method, which is used extensively to describe the electron dynamics in heterojunctions,[3] makes use of the boundary conditions which conserve the probability flux through the heterojunction. The occurrence of a resonance under these boundary conditions is rather obvious. The flux density is determined by the velocity operator, so when the velocity of the incident electron is equal to the velocity of the transmitted electron, the condition for the flux continuity should lead to a situation in which there is no reflected wave ($T=1$). Such a coincidence is possible if the above-the-barrier transition occurs from a broad-band to a narrow-band semiconductor, for example, because of the difference in the effective masses of an electron in the semiconductors of a heterojunction. However, since we are considering heterojunctions with $\Delta_{c,v}\sim E_g$, the single-band method of the effective mass does not hold and the condition under which a resonance can occur should be sought on the basis of a multiband Kane model of an electron spectrum.[4] If the electron momentum along the z axis is zero, the matrix of the Hamiltonian, written in the basis of the eigenfunctions of the momentum, breaks up into two submatrices $H^{(\mu)}$, $\mu=\pm 1$, in accordance with the double degeneration of the volume spectrum. The first row of the submatrix $H^{(\mu)}$ is

$$H_{1i}^{(\mu)} = \{E_g;\ \frac{1}{\sqrt{2}}P\hat{k}_\mu;\ \frac{1}{\sqrt{6}}P\hat{k}_\mu;\ \frac{1}{\sqrt{3}}P\hat{k}_\mu\};\quad \hat{k}_\mu=\hat{k}_x+i\mu\hat{k}_y. \tag{1}$$

The first column is obtained by means of Hermitian conjugation (1). Furthermore, we have $H_{44}^{(\mu)} = -\Delta$ (the parameter of the spin-orbit splitting of the valence band), and all the remaining matrix elements of the Hamiltonian are set equal to zero. We ignore the second-order contribution in the momentum operator $\hat{k}$, since we are considering the electron dynamics only in the conduction band. The flux in this case is of the type characteristic of relativistic problems.[5] It is governed by the nondiagonal elements of the Hamiltonian

$$S_x = \psi_i^+ P_{ij}^{(x)} \psi_j = P\{ \psi_1^* (\frac{1}{\sqrt{2}}\psi_2 + \frac{1}{\sqrt{6}}\psi_3 + \frac{1}{\sqrt{3}}\psi_4) + \text{c. c.} \} . \qquad (2)$$

If the Kane velocity P in the two semiconductors is the same, the boundary conditions which conserve the flux reduce to the continuity ψ_1 and a linear combination of the envelope components in the parentheses. Using (1), we can represent the wave-function envelope as a column with the components

$$\psi^{(\mu)} = \{1; \frac{P\hat{k}_{-\mu}}{\sqrt{2E}}; \quad \frac{P\hat{k}_{\mu}}{\sqrt{6E}}; \quad \frac{P\hat{k}_{\mu}}{\sqrt{3(E+\Delta)}}\} \psi_1(x)\exp(iKy). \qquad (3)$$

Assuming

$$\psi_1(x<0) = C_{\text{incid.}}\exp(ik_1x) + C_{\text{refl.}}\exp(-ik_1x) ; \psi_1(x>0) = C_{\text{trans.}}\exp(ik_2x) ,$$

we find, for example, the following expression for a transmitted wave:

$$S_{x,\text{trans.}} = \frac{2}{3}P^2k_2 |C_{\text{trans.}}|^2 (\frac{2}{E_2} + \frac{1}{E_2+\Delta_2}). \qquad (4)$$

Determining from the boundary conditions the relationship between the amplitudes $C_{\text{incid.}}$ and C_{trans}, we find

$$T = \frac{4r}{(1+r)^2 + q^2} ; \qquad (5)$$

$$r = \frac{k_2E_1(E_1+\Delta_1)(3E_2+2\Delta_2)}{k_1E_2(E_2+\Delta_2)(3E_1+2\Delta_1)} ;$$

$$q = \frac{K}{k_1} \frac{\Delta_1}{(3E_1+2\Delta_1)} [1 - \frac{E_1(E_1+\Delta_1)\Delta_2}{E_2(E_2+\Delta_2)\Delta_1}].$$

This expression should be augmented with Kane's dispersion relations which describe the dispersion of electrons in contact semiconductors

$$P^2(k^2+K^2) = \frac{3E(E-E_g)(E+\Delta)}{3E+2\Delta} \qquad (6)$$

with indices 1 and 2 on the left side and the right side of the boundary, respectively. The resonance transmission is seen most clearly in (4)–(6) at $K=0$ in the limiting cases of the zeroth and the strong ($\Delta_{1,2} = 0, \infty$) spin-orbit coupling. Here $q=0$ and

$r = 1$ ($T = 1$) when the kinetic energy of the transmitted electron, $\varepsilon = E_2 - E_{c2}$, is

$$\epsilon_0 = \frac{E_{g2}\Delta_c}{E_{g1} - E_{g2}}; \qquad E_{g1} > E_{g2}. \tag{7}$$

The longitudinal momentum K does not change qualitatively the behavior of the $T(\varepsilon)$ curve, shifting only the threshold of the above-the-barrier transmission. Figure 1 shows the curves of $T(\varepsilon)$ for the GaAs-GaAlAs, InAs-GaSb, and InAs-InSb heterojunctions. The first heterojunction, which is comprised of wide-band semiconductors, is shown for comparison. In the other two heterojunctions the band gaps at the interface are comparable to $E_{g1,2}$, but the $T(\varepsilon)$ curve diverges from curve 1 in different directions since the last heterojunction satisfies the conditions for the occurrence of a resonance. Here the transmission curve has a jog with $T = 1$, since the spectra of both semiconductors are strongly nonparabolic at energies on the order of ε_0 and the velocities of the incident and transmitted electrons, which are governed by the Kane velocity P, are nearly the same. The dashed curve represents the transmission of an electron with a momentum K along the interface. For comparison, we chose the value of K for each heterojunction so that it would correspond to the energy of the incident electron, $E_1 = E_{g1} + 0.5\Delta_c$, in the case of a purely longitudinal motion. In the case $E_{g1} \gg E_{g2}$ the dependence $T(\varepsilon)$ near ε_0 has a characteristic bell-shaped configuration. We are, however, not aware of any heterojunctions with $\Delta_{c,v} > 0$, which would satisfy this condition.

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Translated by S. J. Amoretty