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Phonon-assisted interband tunnelling in single-barrier structures with type II heterojunctions

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Abstract. The interband tunnelling processes assisted by longitudinal optical (LO) phonons in single-barrier structures with type II heterojunctions are investigated. Kane's model and multicomponent wavefunctions corresponding to the initial and final states are used to obtain the matrix element for interband transition by means of emission of LO phonon inside the barrier. It is shown the phonon-assisted interband tunnelling processes may be dominant even if the transitions without scattering are not forbidden.

Phonon-assisted interband tunnelling may be the main mechanism of carrier interband transition in semiconductor structures made from materials with indirect band gaps [1–3], where the tunnelling processes without scattering are forbidden. This mechanism can provide an interband transition between the quasibound states in double-quantum-well structures, when the levels in different wells are out of resonance [4]. Considerations of the scattering-assisted tunnelling processes in intraband resonant tunnelling structures showed that inelastic tunnelling enhances the current off resonance by orders of magnitude [5, 6]. Here we consider phonon-assisted interband tunnelling at zero temperature in single-barrier structures with type II heterojunctions made from InAs, AlGaSb, GaSb. In structures of this type [7, 8], the narrow-gap materials have direct band gaps. Consequently, the tunnelling processes without scattering are not forbidden, but phonon-assisted tunnelling may play the main role in interband transitions due to the specific band offsets in these heterostructures. In InAs/AlGaSb/GaSb diodes, an electron from the conduction band of the InAs contact layer tunnels through the AlGaSb wide-gap barrier to the valence band of the GaSb contact close to the valence band edge of the barrier. The separation between the InAs conduction band edge and the AlGaSb valence band edge can be of the order of the polar optical phonon energy. Then for all tunnelling electrons the length of penetration into the barrier of the wavefunction corresponding to the final state is greater for phonon-assisted processes than that for tunnelling processes without scattering. We have shown that in this case the phonon-assisted tunnelling may be dominant.

We consider a single-barrier InAs/AlGaSb/GaSb diode under flat-band conditions, whose conduction and valence band diagram is shown in figure 1. The multiband Kane's model [9] is used for investigation of the phonon-assisted interband tunnelling processes. The tunnelling matrix element for the interband transition between the states to the left-hand side of the barrier and to the right-hand side of it by means of emission of a polar optical phonon inside the barrier is calculated using the multicomponent wavefunctions

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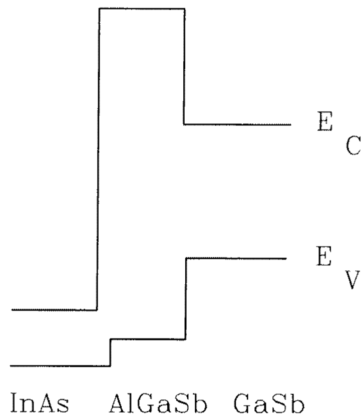

Figure 1. A schematic band diagram of an InAs/AlGaSb/GaSb heterostructure under flat-band conditions.

ψ_l, ψ_r corresponding to the initial and final states. The probability of such a transition per unit time is given by

$$w_{rl} = \frac{2\pi}{\hbar}|M|^2\delta(\bar{E}_r - \bar{E}_l + \hbar\omega) \tag{1}$$

where $\bar{E}_{l,r}$ are the energies of initial and final states, respectively, $\hbar\omega$ is the LO phonon energy, and M is the matrix element. Using the Hamiltonian of the electron–phonon interaction (see, for example, reference [5]), and supposing that normalizing lengths are equal to unity, we obtain

$$|M|^2 = \frac{2\pi e^2}{\bar{\kappa}q^2}\hbar\omega|f|^2. \tag{2}$$

In equation (2), $\bar{\kappa}^{-1} = \kappa_\infty^{-1} - \kappa_0^{-1}$, where κ_0, κ_∞ are the static and high-frequency-limit permittivities, e is the electron charge, $\boldsymbol{q}$ is a phonon wavevector, and the function f is given by

$$f = \delta_{\boldsymbol{k}_{r\parallel},\boldsymbol{k}_{l\parallel}-\boldsymbol{q}_\parallel}\sum_j\int_{-d/2}^{d/2}\mathrm{d}y\ \psi_{rj}^*(y)\exp(-\mathrm{i}q_y y)\psi_{lj}(y). \tag{3}$$

Here y is the direction normal to the interfaces, $y = 0$ in the centre of the barrier, and d is the barrier thickness. We have utilized the normalized wavefunctions ψ_l, ψ_r with components $\bar{\psi}_{lj} = \psi_{lj}(y)\exp(\mathrm{i}\boldsymbol{k}_{l\parallel}\cdot\boldsymbol{r}_\parallel)$, $\bar{\psi}_{rj} = \psi_{rj}(y)\exp(\mathrm{i}\boldsymbol{k}_{r\parallel}\cdot\boldsymbol{r}_\parallel)$ corresponding to the initial and final states with wavevectors $\boldsymbol{k}_{l,r}$.

We use the same basis functions as in reference [10], and the approximations of the transfer Hamiltonian approach [11] to calculate the normalized wavefunctions for the states to the left-hand and to the right-hand side of the barrier layer. Suppose that the lateral wavevector of the incident electron is equal to zero, and the x-axis is parallel to the lateral wavevector of the LO phonon $\boldsymbol{q}_\parallel$. Then the 8×8 Kane's Hamiltonian can be written in the following form [10]:

$$\hat{H} = \begin{pmatrix} \hat{H}_+ & 0 \\ 0 & \hat{H}_- \end{pmatrix} \tag{4}$$

where

$$\hat{H}_{\pm} = \begin{pmatrix} E_C(y) & P\hat{k}_{\pm} & P\hat{k}_{\mp}/\sqrt{3} & \sqrt{2}P\hat{k}_{\mp}/\sqrt{3} \\ P\hat{k}_{\mp} & E_V(y) & 0 & 0 \\ \sqrt{2}P\hat{k}_{\pm}/\sqrt{3} & 0 & E_V(y) & 0 \\ \sqrt{2}P\hat{k}_{\pm}/\sqrt{3} & 0 & 0 & E_V(y)-\Delta(y) \end{pmatrix}. \tag{5}$$

In (5),

$$\hat{k}_{\pm} = \mp \mathrm{i}(\hat{k}_x \pm \mathrm{i}\hat{k}_y)/\sqrt{2}$$

and $E_C(y)$ and $E_V(y)$ are the conduction and valence band edges, $\Delta(y)$ is the split-off energy, and P is proportional to the interband momentum matrix element. We have neglected the term $\hbar^2\hat{k}^2/(2m_0)$ in H_{ii}, where m_0 is the free-electron mass, supposing that m_0 is much greater than the electron or light-hole effective mass. The multicomponent wavefunction ψ_l (ψ_r) satisfies the Schrödinger equation

$$\sum \hat{H}_{ij}\bar{\psi}_{kj} = \bar{E}_k\bar{\psi}_{ki} \qquad i = 1, \ldots, 8;\ k = l\ (r) \tag{6}$$

with the Hamiltonian given by (4), (5) inside the barrier and to the left (right) of the barrier layer, and vanishes to the right (left) of it.

The envelope functions $\bar{\psi}_{lj}$, $\bar{\psi}_{rj}$ can be calculated using equations (4)–(6) and the same boundary conditions as in reference [10]. Supposing that only the first four envelope functions or the last four envelope functions are not equal to zero, only one matrix $\hat{H}_+$ or $\hat{H}_-$ needs to be employed. Note that these matrices define the solutions of the Schrödinger equation with different average values of the spin. The procedure of wavefunction normalization, in which the barrier region can be neglected, is similar to that used in reference [12]. For structures under flat-band conditions, the envelope functions within the barrier are given by

$$\begin{aligned} \psi_{lj}(y)\exp(\mathrm{i}\boldsymbol{k}_{l\parallel}\cdot\boldsymbol{r}_{\parallel}) &= \psi_{lj}(-d/2+0)\exp(-\kappa(y+d/2)) \\ \psi_{rj}(y)\exp(\mathrm{i}\boldsymbol{k}_{r\parallel}\cdot\boldsymbol{r}_{\parallel}) &= \psi_{rj}(d/2-0)\exp(\kappa'(y-d/2)+\mathrm{i}k_{r\parallel}x) \end{aligned} \tag{7}$$

where κ, κ' are the reciprocal lengths of wavefunction penetration into the barrier corresponding to the initial and final states, respectively. Then equation (3) for the function f can be rewritten as

$$\begin{aligned} f = \delta_{\boldsymbol{k}_{r\parallel},\boldsymbol{k}_{l\parallel}-\boldsymbol{q}_{\parallel}} & \sum_j (\psi^*_{rj}(d/2-0)\psi_{lj}(-d/2+0))\exp(-(\kappa+\kappa')d/2) \\ & \times \frac{2\cos(q_y d/2)\sinh((\kappa-\kappa')d/2) + 2\mathrm{i}\sin(q_y d/2)\cosh((\kappa-\kappa')d/2)}{\mathrm{i}q_y + \kappa - \kappa'}. \end{aligned} \tag{8}$$

In the following consideration of the phonon-assisted tunnelling probability, for the sake of simplicity we suppose that $q_{\parallel}$ is much less than the reciprocal length κ' of the penetration of the wavefunction ψ_r into the wide-gap barrier with sufficiently large light-hole effective mass. This assumption is reasonable, because the matrix element of the electron–phonon interaction in equation (2) drastically decreases with phonon wavevector increase. For this reason, intravalley scattering by polar optical phonons has a small-angle character as shown by simulations performed using the Monte Carlo method [13]. We do not take into account the intervalley scattering processes, which produce large-angle scattering events [13], because the energy separation between the Γ valley and upper valleys in the conduction band of InAs is sufficiently large. Note that we do not employ any assumptions as to the values of q_y/κ', $q_\parallel/k_r$, q_y/k_r, because the results can easily be obtained without these assumptions. Then using (4)–(7) we obtain

$$\sum_j (\psi_{rj}^*(d/2-0)\psi_{lj}(-d/2+0))$$
$$= \psi_{rs}^*(d/2-0)\psi_{ls}(-d/2+0)\left(1 - \frac{2P^2\kappa\kappa'}{3(E_b+E_{gb})(E_b+E_{gb}-\hbar\omega)} - \frac{P^2\kappa\kappa'}{3(E_b+E_{gb}+\Delta_b)(E_b+E_{gb}+\Delta_b-\hbar\omega)}\right). \tag{9}$$

Here: E_b is the difference between the incident particle energy and the position of the conduction band edge of the barrier layer with energy gap E_{gb} and split-off energy Δ_b; ψ_{ls}, ψ_{rs} are the envelope functions which correspond to the s-type basis function; and the energy E_b and imaginary wavevector iκ ($E_b - \hbar\omega$ and iκ') satisfy Kane's dispersion relation [9]

$$E(E+E_g)(E+E_g+\Delta) = P^2k^2(E+E_g+2\Delta/3). \tag{10}$$

In equation (10), E and k are the particle energy and wavevector, respectively (the conduction band edge is the energy reference), and E_g and Δ are the energy gap and split-off energy. The spin orientation of the tunnelling electron is not important, because its lateral wavevector is supposed to be equal to zero [14]. In the calculation of κ' we neglect motion lateral to the interfaces. It is possible for $q_\parallel \ll \kappa'$, if $q_\parallel d \times q_\parallel/(2\kappa') < 1$. Then the exponential factor in equation (8) does not depend strongly on $q_\parallel$. If the volume of normalization is equal to unity, then the envelope functions $\psi_{ls}(-d/2+0)$ and $\psi_{rs}(d/2-0)$ inside the barrier satisfy the following equations:

$$|\psi_{ls}(-d/2+0)|^2 = 4\left[1+\frac{E_b^2k_l^2}{E_l^2\kappa^2}\right]^{-1}\left[1+\frac{2P^2k_l^2}{3(E_l+E_{gl})^2}+\frac{P^2k_l^2}{3(E_l+E_{gl}+\Delta_l)^2}\right]^{-1} \tag{11}$$

$$|\psi_{rs}(d/2-0)|^2 = 4\left[1+\frac{(E_b-\hbar\omega)^2k_r^4}{E_r^2k_{yr}^2\kappa'^2}\right]^{-1} \times \left[1+\frac{2P^2k_r^2}{3(E_r+E_{gr})^2}+\frac{P^2k_r^2}{3(E_r+E_{gr}+\Delta_r)^2}\right]^{-1}. \tag{12}$$

Here $E_{l,r}$ are the energies of initial and final states, while the conduction band edge is the energy reference at each point, E_{gl}, E_{gr} are the energy gaps of the contact layers, $\Delta_{l,r}$ are the split-off energies of these layers, and E_l (E_r) and k_l (k_r) satisfy Kane's dispersion law [9]. The dependence of ψ_{rs} upon spin is neglected as in reference [10]. Then the probability of a particle transition from each state in the left-hand contact layer to the right-hand side of the barrier is independent of the orientation of the LO phonon lateral wavevector.

From equations (2), (8), (9) it is obvious that the tunnelling matrix element for the phonon-assisted process can be equal to zero for some transitions, while the tunnelling matrix element for the process without scattering [12] is not equal to zero. The latter contains the exponential factor $\exp(-\kappa d)$, which can be much less than the exponential factor in the right-hand side of equation (8) for incident particle energy close to the barrier layer valence band edge if $\kappa d \gg 1$, because $\kappa' < \kappa$. For this reason the phonon-assisted tunnelling probability in the InAs/AlGaSb/GaSb diodes with sufficiently thick barrier layers may be greater than that for tunnelling processes without scattering.

The phonon-assisted tunnelling probability T is obtained using the tunnelling matrix element M defined by (2), (3) in a way similar to that described in reference [12]. It is equal to the total transition rate divided by the probability flux density in the incident wave. The total transition rate is calculated by summing the transition rate (1) over all phonon wavevectors and all final states in the valence band, and is given by

$$W_{rl} = \frac{2\pi}{\hbar} \sum_{\boldsymbol{q},k_r} |M|^2 \delta(\bar{E}_r - \bar{E}_l + \hbar\omega). \tag{13}$$

Replacing the sum with an integral, we obtain

$$W_{rl} = \frac{1}{(2\pi)^3\hbar} \int \mathrm{d}^3q \; |M|^2 \, \partial k_{yr}/\partial E_r \tag{14}$$

where $\bar{E}_r = \bar{E}_l - \hbar\omega$, $k_{yr}^2 + q_\parallel^2 = k_r^2$; if the electron tunnels to the valence band, the sign of the product $k_{yr} \times k_{yl}$ should be negative. In equation (14)

$$\partial k_{yr}/\partial E_r = \frac{k_r^2}{2E_r k_{yr}} \left[1 + \frac{2P^2k_r^2}{3(E_r + E_{gr})^2} + \frac{P^2k_r^2}{3(E_r + E_{gr} + \Delta_r)^2}\right]. \tag{15}$$

The probability flux density in the incident wave j_I is given by [12]

$$j_I = \frac{2E_l}{\hbar k_l} \left[1 + \frac{2P^2k_l^2}{3(E_l + E_{gl})^2} + \frac{P^2k_l^2}{3(E_l + E_{gl} + \Delta_l)^2}\right]^{-1}. \tag{16}$$

Using equations (14)–(16) and the matrix element for the LO phonon-assisted tunnelling process defined by (2), (8)–(12), the expression for the tunnelling probability $T = W_{rl}/j_I$ can be written as

$$\begin{aligned} T = {} & \frac{4\hbar\omega e^2}{\pi\bar{\kappa}} \exp\left(-(\kappa + \kappa')d\right)\left(1 + \frac{E_b^2 k_l^2}{E_l^2 \kappa^2}\right)^{-1} \frac{k_l k_r^2}{E_l |E_r|} F \\ & \times \left(1 - \frac{2P^2\kappa\kappa'}{3(E_b + E_{gb})(E_b + E_{gb} - \hbar\omega)}\right. \\ & \left. - \frac{P^2\kappa\kappa'}{3(E_b + E_{gb} + \Delta_b)(E_b + E_{gb} + \Delta_b - \hbar\omega)}\right)^2. \end{aligned} \tag{17}$$

Here

$$F = 2\int_0^\infty \mathrm{d}q_y \; F_0 \frac{\cos^2(q_y d/2)\sinh^2((\kappa - \kappa')d/2) + \sin^2(q_y d/2)\cosh^2((\kappa - \kappa')d/2)}{q_y^2 + (\kappa - \kappa')^2} \tag{18}$$

where the upper limit of the integral is extended to infinity, and the function $F_0(q_y^2)$ is given by

$$\begin{aligned} F_0(q_y^2) = {} & \left(\sqrt{k_r^2 + q_y^2}\,\ln\left(\frac{\sqrt{k_r^2 + q_y^2} + k_r}{\sqrt{k_r^2 + q_y^2} - k_r}\right) - 2\left|\frac{(E_b - \hbar\omega)k_r^2}{E_r\kappa'}\right| \arctan\left|\frac{E_r\kappa'}{(E_b - \hbar\omega)k_r}\right|\right) \\ & \times \left(\left(\frac{(E_b - \hbar\omega)k_r^2}{E_r\kappa'}\right)^2 + k_r^2 + q_y^2\right)^{-1}. \end{aligned} \tag{19}$$

Equations (17)–(19) can be used also for the description of the phonon-assisted intraband tunnelling processes. If for the initial state $E_l < 0$, then k_l in equation (17) should be negative. The phonon-assisted interband tunnelling probability in the InAs/$Al_xGa_{1-x}Sb$/GaSb diode ($x \approx 0.4$) with barrier thickness equal to 20 nm versus the incident electron energy calculated using equations (17)–(19) is shown in figure 2 (curve 1). For comparison, the interband tunnelling probability calculated using the expression presented in reference [10] versus the incident electron energy for the process without

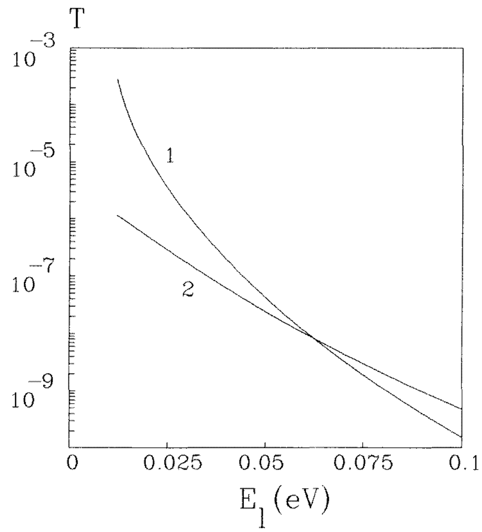

Figure 2. The phonon-assisted interband tunnelling probability (curve 1) and the interband tunnelling probability for the process without scattering (curve 2) versus the electron incident energy.

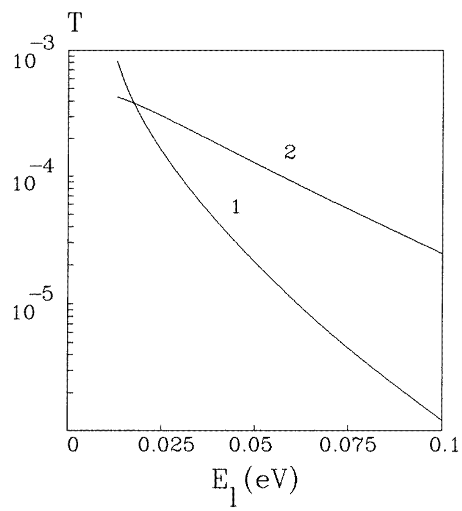

Figure 3. The tunnelling probability in an InAs/AlGaSb/GaSb diode with a 10 nm barrier layer.

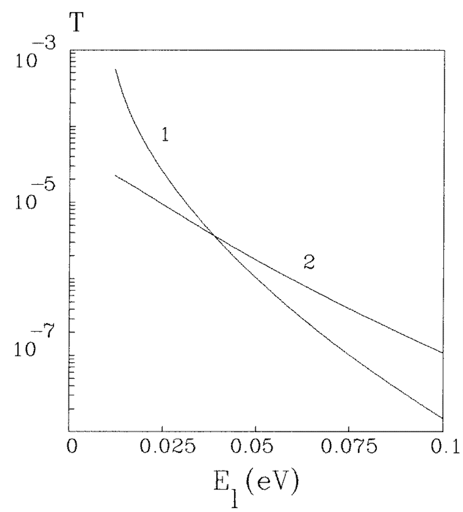

Figure 4. The tunnelling probability in an InAs/AlGaSb/GaSb diode with a 15 nm barrier layer.

scattering is shown in this figure too. We have used the same parameters as in reference [15]. The calculations show that the phonon-assisted tunnelling is dominant for particle energy close to the valence band edge of the barrier. The tunnelling probability with scattering inside the barrier is several orders of magnitude greater than that for the process without scattering for energies of the order of 10 meV. The tunnelling probabilities both for inelastic processes and for processes without scattering drop as the energy increases, due to the decreasing of the lengths of wavefunction penetration into the barrier. The

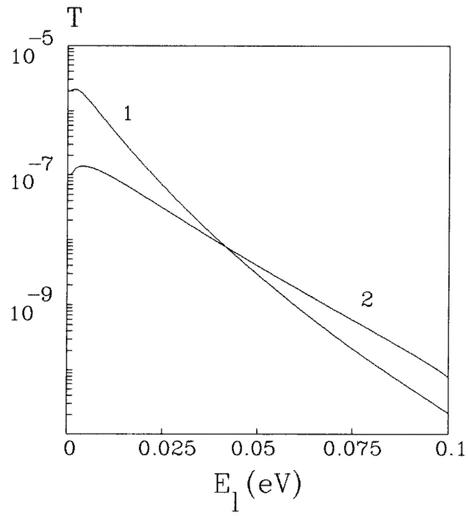

Figure 5. The tunnelling probability versus incident particle energy in an InAs/AlGaSb/GaSb diode under bias.

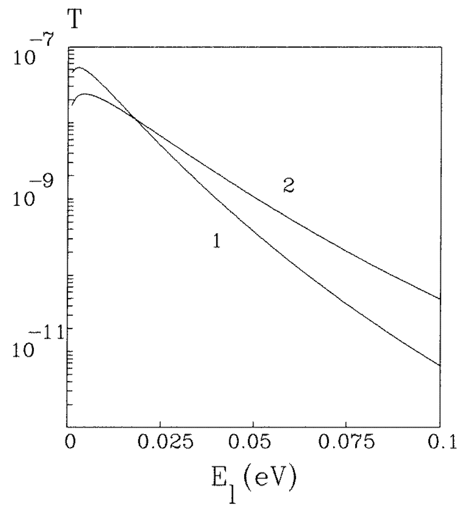

Figure 6. The tunnelling probability versus incident particle energy in an InAs/AlGaSb/InAs diode under bias.

values of T for incident energies corresponding to final energies less than the position of the valence band edge of the barrier are not shown in figure 2, because the approximations used are not valid in this region of parameters. It is clear that the results will not change qualitatively in this case. To demonstrate the barrier thickness dependence of the phonon-assisted tunnelling probability, we have calculated the values of T for structures with barrier thickness $d = 10$ nm and $d = 15$ nm. (See figures 3 and 4, respectively, where curves 1, 2 are as in figure 2.) The calculations showed that the role of the phonon-assisted tunnelling decreases with the decrease of the barrier thickness, and is not very important if $d < 10$ nm.

It should be noted that in InAs/AlGaSb/InAs structures under flat-band conditions, phonon-assisted tunnelling processes are not so important as in InAs/AlGaSb/GaSb structures, because of a sufficiently small density of final states near the conduction band edge of the right-hand InAs layer. These processes may be dominant in InAs/AlGaSb/InAs structures if the separation between the InAs conduction band edge and the AlGaSb valence band edge is close to zero, or if an external bias is applied to the diode. If the right-hand InAs contact layer is positively biased, then the density of states in this layer for all electrons tunnelling from the left-hand InAs layer enlarges. As a result, the ratio of the phonon-assisted tunnelling probability and the tunnelling probability for the process without scattering for energies close to barrier layer valence band edge can increase. Equations (17)–(19) allow us to evaluate the tunnelling probability assisted by LO phonons in a structure under bias in a similar way to references [5, 6]. In this procedure of tunnelling probability calculation, the potential inside the barrier is supposed to be constant, while the conduction band discontinuity for the left-hand heterojunction is reduced by $|e|V/2$ and the discontinuity for the right-hand heterojunction is increased by $|e|V/2$, where V is the voltage across the barrier layer. The dependencies of the tunnelling probability on the energy of incident electrons in the InAs layer for InAs/AlGaSb/GaSb, InAs/AlGaSb/InAs diodes with 20 nm barriers under the bias of 0.04 V are shown in figures 5 and 6, respectively. Curve 1 in each figure corresponds to the tunnelling process assisted by LO phonons, and curve 2 corresponds to the process without scattering. The phonon-assisted tunnelling processes are dominant for low incident particle kinetic energies in both structures under bias.

In the calculations of the phonon-assisted tunnelling probability, for the sake of simplicity we considered the 3D phonon modes, while in real multilayer structures, due to the difference in lattice parameters, such polar optical phonon modes occur as interface, slab, and half-space modes [16]. Consideration of the coupling of the electrons and optical phonons in GaAs/AlGaAs quantum wells [16] showed that the contribution of the confined slab phonon modes in the polaron binding energy and effective mass is dominant for quantum well widths greater than 10 nm, because the lengths of penetration into the slab of the half-space and interface modes are sufficiently small. For this reason the contribution of the slab phonon modes to the phonon-assisted tunnelling probability should also be dominant in single-barrier structures with thick barriers. For $d = 20$ nm, the minimum value of q_y for the slab mode is about 10^6 cm^{-1}, which is essentially less than the characteristic reciprocal lengths of electron wavefunction penetration into the barrier layer. In this case, consideration of the phonon quantization effects will not change the results very much. If the phonon temperature is not equal to zero, the processes with emission and absorption of LO phonons may both occur. The role of the processes with LO phonon absorption is not essential in the structures under consideration, because the length of penetration into the barrier of the wavefunction corresponding to the final state decreases as the energy increases, due to LO phonon absorption. The contribution of the processes with LO phonon emission is greater by a factor of $1 + N$, where N is the occupation of phonon states, in the case of finite temperature than that at zero temperature.

In summary, we have shown that the phonon-assisted interband tunnelling in structures with type II heterojunctions and thick barriers may be dominant for incident particle energy close to the valence band edge of the barrier layer. Consequently, phonon-assisted tunnelling can define the current density in the structures with type II heterojunctions, which contain sufficiently thick barriers.

References

[1] Keldysh L V 1958 *Sov. Phys.–JETP* **6** 763
[2] Keldysh L V 1959 *Sov. Phys.–JETP* **7** 665
[3] Kane E O 1961 *J. Appl. Phys.* **32** 83
[4] Aleiner I L and Luberton J P 1995 *Appl. Phys. Lett.* **67** 1423
[5] Wu G Y and McGill T C 1989 *Phys. Rev.* B **40** 9969
[6] Chevoir F and Vinter B 1989 *Appl. Phys. Lett.* **55** 1859
[7] Luo L F, Beresford L R and Wang W I 1989 *Appl. Phys. Lett.* **55** 2023
[8] Södeström J R, Chow D H and McGill T C 1989 *Appl. Phys. Lett.* **55** 1348
[9] Kane E O 1957 *J. Phys. Chem. Solids* **1** 249
[10] Zakharova A, Ryzhii V and Pesotzkii V 1994 *Semicond. Sci. Technol.* **9** 41
[11] Bardeen J 1961 *Phys. Rev. Lett.* **6** 57
[12] Zakharova A and Gergel V 1995 *Solid State Commun.* **96** 209
[13] Fawcett W, Boardman A D and Swain S 1970 *J. Phys. Chem. Solids* **31** 1963
[14] Zakharova A, Vasko F T and Ryzhii V 1994 *J. Phys.: Condens. Matter* **6** 7537
[15] Ryzhii V and Zakharova A 1992 *Semicond. Sci. Technol.* **7** 980
[16] Hai G Q, Peeters F M and Deveese J T 1993 *Phys. Rev.* B **48** 4666