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Boundary conditions for the heterojunction interfaces of nonparabolic semiconductors

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Transmission probability curves are presented for $InAs/Al_{0.4}Ga_{0.6}Sb/InAs$ tunnel diodes which show that for a 2-nm-barrier width, negative differential conductance (NDC) is indicated if the velocity effective mass is used to match the derivatives of the wave functions at the heterojunction interfaces, while the use of the energy-effective mass does not indicate an NDC. It is suggested that an experiment with such a diode may resolve the controversy about the effective mass, to be used for matching the derivatives.

The nonparabolicity of energy bands plays an important role in determining the energy eigenvalues and tunneling probability in type II, heterostructures, since in such structures the conduction band edge of one layer is very near the valence band edge of the other layer. The observed negative differential conductance[1,2] in $InAs/Al_xGa_{1-x}Sb/InAs$ tunnel diodes has, in fact, been explained to be due to the nonparabolic energy-wave-vector (E-k) relation in the forbidden band of $Al_xGa_{1-x}Sb$. Preliminary calculations by using the Wentzel–Kramers–Brillouin (WKB) approximation to evaluate the tunneling probability have been reported to fit the experimental data.

It may, however, be noted that a proper evaluation of the transmission probability of the electrons requires the solution of the wave equation to take account of the reflections that occur at the potential discontinuities. The boundary conditions to be used for the solution has been controversial for nonparabolic bands as explained below.

Solution of the wave equation for the ith layer is taken as

$$\psi_i = F_i(z)\exp(i\mathbf{k}_{ti}\cdot\boldsymbol{\rho}), \tag{1}$$

where $F_i(z)$ is the envelope function, $\mathbf{k}_{ti}$ and $\boldsymbol{\rho}$ are, respectively, the in-plane component of the wave vector and the position vector.

The boundary conditions satisfied by the wave functions at the discontinuities are:

$$\begin{aligned}&(i)\,\psi_i=\psi_{i+1},\\ &(ii)\,(1/m_i)(\partial/\partial z)\psi_i=(1/m_{i+1})(\partial/\partial z)\psi_{i+1}.\end{aligned} \tag{2}$$

The first condition ensures the continuity of probability density and leads to the result that k_t is continuous across the interface. It is, however, assumed that $k_{ti}=0$ as it is not relevant to the present discussion.

The second condition ensures the continuity of probability current density. For parabolic bands, m_i, m_{i+1} are the band-edge effective masses for the ith and the $(i+1)$th layer. The controversy is about which mass should be used for nonparabolic bands, since nonparabolic E-k relation admits three effective masses, the energy-effective mass, the velocity- or optic-effective mass, and the acceleration-effective mass, which are given, respectively, by $(\hbar^2k^2/2E)$, $(\hbar^2k/\nabla_kE)$, and $(\hbar^2/\nabla_k^2E)$. The energy-effective mass has been used in the past[3] for m_i. It does not, however, ensure the continuity of probability current density, which must be satisfied in the steady state.

Nag and Mukhopadhyay[4] suggested that the velocity-efective mass should be used in condition (2) (ii) to ensure continuity of probability current density and found that the band offset in $InP/Ga_{0.47}In_{0.53}As$ system obtained by using this mass in the photoluminescence data, is in agreement with the value, determined by other methods. That the velocity-effective mass is appropriate may also be proved as follows. The effective-mass equation for $F_i(z)$ may be shown[5] to be given by

$$E(-i\nabla)F_i(z)+(E-E_{ci})F_i(z)=0, \tag{3}$$

where E is the total energy and E_{ci}, the band edge energy of the electron. The operator $E(-i\nabla)$ is obtained by replacing k in the expression for $E(k)$ by $-i\nabla$; in the present case $\nabla\equiv\partial/\partial z$. A general expression for $E(k)$ may be taken to be

$$E=E_c+\sum_{n=1}^{\infty}a_nk^{2n}. \tag{4}$$

For example, the Kane 3-band $k\cdot p$ E-k relation,

$$\hbar^2k^2/2m^*=(E-E_c)[1+\alpha(E-E_c)], \tag{5}$$

may be expressed as

$$E=E_c+a_1k^2-\alpha a_1^2k^4+2\alpha^2a_1^3k^6-,..., \tag{6}$$

with $a_1=\hbar^2/2m^*$.

By using the operator $E(-i\nabla)$ corresponding to Eq. (4) in Eq. (3) and considering that $F_i(z)$ is of the form of $\exp(ikz)$, it may be easily shown that

$$\sum_{n=1}^{\infty}a_nk^{2(n-1)}[F_i(z)\partial_zF_i^*(z)-F_i^*(z)\partial_zF_i(z)]=\text{constant}. \tag{7}$$

In other words,

$$(1/\hbar^2k)\partial_kE[F_i(z)\partial_zF_i^*(z)-F_i^*(z)\partial_zF_i(z)]=\text{constant}. \tag{8}$$

Since F is continuous across the interface, this result shows that the velocity-effective mass, $m_v(E)$, given by $(\hbar^2k/\nabla_kE)$ should be used in (2) (ii).

The use of the two masses, the energy-effective mass or the velocity-effective mass, however, do not give significantly different properties for type I heterojunctions, like $GaAs/Al_xGa_{1-x}As$, $Al_{0.48}In_{0.52}As/Ga_{0.47}In_{0.53}As$ or $InP/Ga_{0.47}In_{0.53}As$, since the conduction band offset is smaller than the halfwidth of the forbidden band in barrier layers of such systems. Calculations indicate differences of less than 10% in the measured parameter, which may also be due to uncertainties in the values of various physical constants and structural parameters. The controversy cannot, therefore, be resolved by experiments on these systems.

The transmission probability for an $InAs/Al_xGa_{1-x}Sb/InAs$ system is, however, found to be qualitatively different when the energy or the velocity effective mass is used in condition (2) (ii).

Transmission probability is obtained for a single barrier of width d from the following expressions for the envelope functions in the incident layer F_i, in the barrier layer F_B, and in the outgoing layer F_0.

$$F_i = \exp(ik_1z) + R\exp(-ik_1z), \quad (9)$$

$$F_B = A\exp(ik_2z) + B\exp(-ik_2z), \quad (10)$$

$$F_0 = T\exp(ik_3z), \quad (11)$$

where

$$k_i^2 = (2m_i/\hbar^2)\gamma(E - E_{ci}), \quad (i=1,2,3). \quad (12)$$

The nonparabolic energy function is indicated by $\gamma(E - E_{ci})$, which is $(E - E_{ci})[1 + \alpha(E - E_{ci})]$ in the Kane relation. An electron wave of unit amplitude with energy E is assumed to be incident on the barrier. R and T are, respectively, the reflection and the transmission coefficients. A and B are unknown constants. T may be evaluated by solving Eqs. (9)–(11), by using the boundary condition of (2).

The transmission probability, T_P, being defined as the ratio of the outgoing electron flux to the incoming flux is found to be given by

$$T_P = (m_{v1}/m_{v3})\cdot(m_3/m_1)4ab[(a+b)^2\cos^2 k_2d - (ab-1)^2\sin^2 k_2d]^{-1}, \quad (13)$$

where $a = k_2m_1/k_1m_2$, $b = k_2m_3/k_3m_2$, $m_{vi}(i = 1,3)$ is the velocity-effective mass in the ith layer. $m_i(i = 1,2,3)$ is either the energy-effective mass $m_i(E - E_{ci})^{-1}\gamma(E - E_{ci})$ or the velocity-effective mass $m_i\partial_E[\gamma(E - E_{ci})]$.

Transmission probability was computed for the $InAs/Al_{0.4}Ga_{0.6}Sb/InAs$ system, on which experiments have been reported.[1,2] Physical constants were taken as follows:

$$m_1^* = m_3^* = 0.023m_0;\ m_2^* = 0.091m_0;\ m_0 = 9.1\times10^{-31}\ \text{kg},$$

$$E_{c2} - E_{c1} = E_{c2} - E_{c3} = 1250\ \text{meV};$$

The Kane relation[6] was assumed to describe the nonparabolicity as in the earlier studies[1,2] and the values of the nonparabolicity parameters were taken as

$$\alpha_1 = \alpha_3 = 2.8\ \text{eV}^{-1}, \quad \alpha_2 = 0.78\ \text{eV}^{-1}.$$

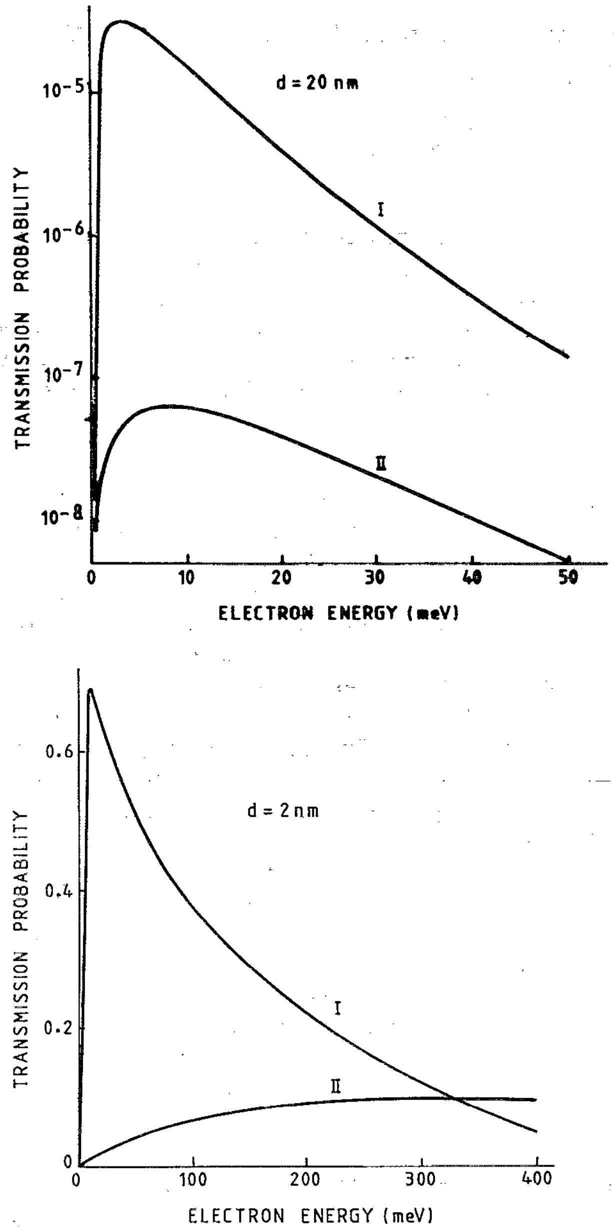

FIG. 1. Transmission probability in $InAs/Al_{0.4}Ga_{0.6}Sb/InAs$ tunnel diode. I—Probability obtained by using the velocity effective mass in the boundary condition. II—Probability obtained by using the energy effective mass in the boundary condition. Barrier width: (a) 2 nm; (b) 20 nm.

Computed transmission probability characteristics are shown in Fig. 1 for the barrier widths of 20 and 2 nm.

It is seen that for the width of 20 nm, both the effective masses give transmission probabilities which initially increase with energy, but after showing a peak, decrease with energy up to about 600 meV. The probability increases again for further increase in energy. This part is not shown as it is not relevant to the present discussion. It is also seen that though the two curves have similar features, the magnitude of the transmission probability is an order higher for the velocity-effective mass curve. The decrease of transmission probability with energy produces negative differential conductance (NDC) of the diodes, which has been confirmed by calculating the current-voltage characteristics. Use of both the masses thus indicates NDC for the diodes but of different magnitudes. It will be difficult to resolve the controversy by experiments on such diodes as the uncertainties in the values of different physical constants and experimental parameters may mask the difference.

The transmission probability curves for a barrier width of 2 nm are, however, radically different in nature. While the curve obtained with the velocity-effective mass has a region in which T_P decreases sharply with energy, the curve for the energy-effective mass has no such region. One may conclude that if the right mass for the boundary condition is the energy-effective mass, no NDC will be seen in diodes with a barrier width of 2 nm. Calculations indicate that this result will be applicable for widths smaller than 3 nm. On the other hand, if velocity effective mass is the right mass, then NDC will be observed for all barrier widths.

In conclusion, experiments with $InAs/Al_{0.4}Ga_{0.6}Sb/InAs$ diodes of barrier widths less than 3 nm would settle the controversy about which effective mass, energy or velocity-effective mass, should be used to match the derivatives of wave functions at the potential discontinuities in nonparabolic heterostructures.

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