Resonant tunneling through traps in Schottky barriers
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To cite this version:

HAL Id: jpa-00208717
https://hal.archives-ouvertes.fr/jpa-00208717
Submitted on 1 Jan 1977

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1. Introduction. — The role that impurities play in tunneling effects in barriers has been discussed by a number of authors [1-10]. In the case of Schottky barriers two main effects have been distinguished:

i) The barrier shape is altered by the presence of ionized impurities and as a consequence the direct tunneling effect is enhanced [10].

ii) The impurity levels resonate with electrons in both the metal and the semiconductor; this effect also causes an enhancement of the tunneling mechanism [2-7]. In an earlier paper [9] the resonant tunneling problem was tackled by applying a phenomenological formalism analogous to that of Hall-Schockley and Read, first applied by G. H. Parker and C. A. Mead [6] to the case of tunneling through traps. In this context the probability of both the trap-semiconductor and the metal-semiconductor transitions were accurately computed. The assumption that the whole physical transition connecting the metal to the semiconductor through a trap could be split into these two independent mechanisms was, of course, implied.

Recently, however, A. V. Chaplik et al. [4] put forward some objections to this type of approach, according to these authors the physical phenomena involved cannot be separated into two independent mechanisms. Indeed, doing this neglects the width of the trap level that arises by tunneling. We show in the present paper that as far as deep level impurities are concerned, considering the width of the level does not alter the quantitative results obtained in the framework of the phenomenological assumptions. The current expressions of both theories tend to the same equation when the impurity level is lowered.

The results obtained are applied to the case of a metal-AsGa barrier. The comparison between the trap assisted and the direct tunneling currents [11] show how efficient trap assisted current may be in the case of such a barrier.

2. The physical formalism. — Let us consider a potential barrier \( U(z) \) that contains an impurity level at \( r_j \), whose potential is \( v(r - r_j) \). We shall neglect any deformation of \( U(z) \) due to the presence of the impurity.

The calculation of the current that goes through the barrier is then conducted in three stages:

1) The wave function of an electron in the whole barrier, including the trap, is determined.
2) The transparency of the barrier is obtained.
3) The current density expression is computed.
We shall, in what follows, describe these three stages.

2.1 THE WAVE FUNCTION. — Under the above mentioned physical conditions A. V. Chaplik et al. [4] showed that the wave function that includes the presence of the trap can be written:

\[ \psi(r) = \psi_0(r) + \left[ E - E_0' - \frac{\Gamma}{2} \right]^{-1} \times \int dr_1 g(r, r_1) v(r_1 - r) \varphi(r_1 - r) \]
\[ \times \int dr_2 v(r_2 - r) \varphi(r_2 - r) \psi_0(r_2) \]  \hspace{1cm} (1)

where \( \psi_0(r) \) represents the wave function of the electron if not trap effect were included, \( E \) the electron energy, \( E_0' \) the trap level, \( \Gamma \) the perturbation of the trap energy level due to the presence of a continuous spectrum, \( \varphi(r) \) the wave function of the trapped electron. In figure 1 the shape of the wavefunctions \( \psi(r) \), \( \psi_0(r) \) and \( \varphi(r) \) have been represented for values of \( E \) close to \( E_0' \).

When no trap is included in the barrier the corresponding wavefunction dies out exponentially within the barrier and is highly attenuated at the output. The presence of the trap brings about the resonance phenomenon. A quasi-stationary wave of large amplitude is built up inside the trap and both exponentially increasing and decreasing waves are created in the forbidden region thus allowing large transmittivities.

\[ g(r, r') \] stands for the barrier Green function and we then have:

\[ (H_0 + U(z) - E) g(r, r') = -\delta(r - r') , \]
\[ H_0 = -\frac{\hbar^2}{2m} \nabla^2 \]  \hspace{1cm} (2)

where \( m \) is the electron effective mass.

Eq. (1) holds when \( E - E_0' < \Delta \), where \( \Delta \) represents the difference between two successive energy levels of the trap; in the case of a resonant tunneling problem, \( E_0' \) represents the ground state.

It is then necessary to provide the trap with a representation of its potential. It appears that a Dirac \( \delta \) function is suitable. Indeed, S. Pantelides et al. [12] showed that the potential of a non isochoric impurity is confined within several atomic lengths. Furthermore, numerous authors have obtained close agreement between theory and experiment by using such a \( \delta \) model [13-16].

Under these circumstances eq. (1) becomes:

\[ \psi(r) = \psi_0(r) + \left[ E - E_0' - \frac{\Gamma}{2} \right]^{-1} \times \]
\[ \psi_0(r) \left[ v(r) \varphi(r) \right]_{E_0'}^{E_0} g(r, r') . \]  \hspace{1cm} (3)

The trap energy level perturbation \( \Gamma \) is a complex number [17]. Its real part represents the level shift; this is of no physical interest here and can be included in \( E_0' \); its imaginary part accounts for the level width and is brought about by the transition of a trapped electron into the electrode continuous spectrum. This imaginary part, that we shall still denote \( \Gamma \), is linked to the finite lifetime of the trapped electron and can be determined from the transition probabilities \( T_L \) and \( T_R \) of the electron towards the electrodes. From Heisemberg’s uncertainty relationship we get:

\[ \Gamma = \hbar (T_L + T_R) \]  \hspace{1cm} (4)

the two transition probabilities \( T_L \) and \( T_R \) can be determined by the transfer Hamiltonian Method (18), their expression will be given later.

2.2 THE TRANSPARENCY OF THE BARRIER. — The barrier Green’s function can be determined within the framework of the W.K.B. approximation. As we assume that the \( k \) vector component along the barrier plane will be kept unchanged it is possible to write for the right hand side of the barrier:

\[ g(r, r') = (2\pi)^{-2} \int e^{i\theta - r' - r} g(q, z, z', E) d^3q . \]  \hspace{1cm} (5)

When this equation is substituted into (2) it appears that a one dimensional Schrödinger equation depicts the behaviour of \( g(q, z, z', E) \); its solution takes on the following form:

\[ g(q, z, z', E) = \frac{m}{\hbar^2} \int_{-\infty}^z p_q(x) dx \times \int_{-\infty}^{z'} p_q(x) dx + i\frac{\pi}{4} \]  \hspace{1cm} (5')
with

\[ p_s^2(x) = \frac{2m}{\hbar^2} \left[ E - U(x) \right] - q^2 \quad \text{if} \quad x > a \]

\[ p_s^2(x) = \frac{2m}{\hbar^2} \left( U(x) - E \right) + q^2 \quad \text{if} \quad 0 < x < a \]

where \( a \) is the right classical turning point.

The incident electron wave function has been chosen such that the current density of the incident wave is equal to unity. Applying the current density operator to eq. (3) will then directly provide the barrier transparency.

By using eq. (5) we get [19]:

\[ T(E, k) = (4\pi)^{-1} m^2 \hbar^{-4} \left[ \psi(r) \varphi(r) \right]_{r=0}^{a} \times \]

\[ \times \left[ \int_0^{a} \frac{dx}{p_0(x)} \right]^{-1} \exp \left\{ -\int_0^{a} \frac{dx}{p_0(x)} \right\} \]

\[ \times \exp \left\{ -2 \int_0^{a} \frac{dx}{p_0(x)} \right\} \]

This expression clearly shows the influence upon the transmission amplitude of both the energy \( E \) and the level broadening \( \Gamma \). Indeed, the presence of the term \( (E - E_0)^2 + \Gamma^2/4 \) causes the transmission to go through a maximum when the level broadening is minimum i.e. when \( T_L = T_R \) and for \( E = E_0 \).

In the case of a Dirac \( \delta \) function we have:

\[ \left[ \psi(r) \varphi(r) \right]_{r=0} = (8 \pi^2 \hbar^6 E_0^3 m^{-3})^{1/4} \]

In order to evaluate \( T(E, k) \) completely we still have to get an expression for \( \Gamma \). As explained before this will be determined by the transition probabilities of the trapped electron towards the electrodes. In [9] we justified the use of the transfer Hamiltonian method in the case of a transition connecting the trap to the continuous spectrum. The transition probability, either \( T_L \) or \( T_R \) is:

\[ T_{L,R} = \frac{2\pi}{\hbar} \int d^2k \left| T_{KL} \right|^2 \frac{\partial n}{\partial E} \delta(E - E_0) \]

in which

\[ T_{KL} = \int \psi_0^*(r) \varphi(r) d^3r \]

\( L \) and \( R \) respectively stand for the left and the right electrode, \( \frac{\partial n}{\partial E} \) stands for the state density in the electrode at energy \( E \) and for a constant transverse moment component; \( \psi_0^*(r) \) represents the electron wave in any one of the two electrodes.

This gives, when using the WKB approximation:

\[ \Gamma = \frac{\hbar^2}{2m} \left\{ \int_0^{a} \frac{dx}{p_0(x)} \right\}^{-1} \exp \left\{ -\int_0^{a} \frac{dx}{p_0(x)} \right\} \]

\[ \times \exp \left\{ -2 \int_0^{a} \frac{dx}{p_0(x)} \right\} \]

2.3 THE CURRENT EXPRESSION. — The transparency of the barrier being determined, the density of the current that goes through it will be given by:

\[ j(E_0, z_j) = \frac{(2s + 1) e}{(2\pi)^3} \int \delta(E - f(E + eV)) d^2k T(E, k) \]

in which \( s \) represents the electron spin, \( f(E) \) the occupancy of the energy level \( E \).

After integrating over \( k \) in (9) the current density is given by:

\[ j(E_0, z_j) = \frac{(2s + 1) e}{8\pi} m^{-2} \hbar^3 E_0 \int dE [U(z_j) - E]^{-1} \left[ \int_0^{a} \frac{dx}{p_0(x)} \right]^{-1} \left[ \int_0^{a} \frac{dx}{p_0(x)} \right]^{-1} \]

\[ \times \exp \left\{ -2 \int_0^{a} \frac{dx}{p_0(x)} \right\} \left( E - E_0 \right)^2 + \frac{\Gamma^2}{4} \approx 2\pi \Gamma^{-1} \delta(E - E_0) \]

It appears that the current going through the barrier at energy \( E \) shows a sharp maximum for \( E = E_0 \).

Indeed, if \( \Gamma \ll E_0 \) we have (1):

\[ j(E_0, z_j) = 2 e \frac{T_L T_R}{T_L + T_R} \left( f(E_0) - f(E_0 + eV) \right) \]

then inserting (11) into (10) leads to:

\[ j(E_0, z_j) = 2 e \frac{T_L}{T_L + T_R} \left( f(E_0) - f(E_0 + eV) \right) \]
This result is the same as that obtained when using the detailed balance principle (H-S-R) i.e. when the whole transition is split into its two elementary components. The occupancy of the trap is then obtained by setting the equality between the electrode 1 → trap current and the trap → electrode 2 current.

The identity between these two results is basically linked to the fact that we have used, on the one hand, a potential well represented by a Dirac δ function and, on the other hand, the WKB approximation. It is apparent that these two approximations appear to be convenient in so far as the trap is deep and the barrier is wide enough to have its direct transmission probability at $E_o$ much lower than one. It is worth noticing that, under these circumstances the resonant transmission can reach values close to unity and that this does not mean that the WKB approximation cannot be applied. Indeed, this approximation is used to get $\psi_0(r), \psi_0^*(r), g(r, r')$ and these quantities apply to the barrier containing no impurity.

The main properties exhibited by the current described by eq. (12) are:

i) For a given trap level $E_i, j(E_i, z_j)$ goes through a maximum when $z_j = z_m$ such that $T_L = T_R$.

ii) Another maximum exists related to the fact that the barrier transmission increases with the trap energy whereas the occupancy factor decreases.

3. Application to the case of a Schottky barrier. —

In the case of a Schottky barrier reversely biased the shape of the potential is correctly approximated by:

$$ U(z) = \phi_{BN} - F \cdot z $$

where $\phi_{BN}$ represents the barrier height and $F$ the electric field in the space charge region (see Fig. 1).

The probabilities $T_L$ and $T_R$ are then given by (2)

$$ T_L = 1.483 \times 10^7 \, m^{-1/2} \times$$

$$ \times F \left[ (E_o + F z_j)^{1/2} - E_o^{3/2} \right]^{-1}$$

$$ \times \exp \left[ - \beta [(E_o + F z_j)^{3/2} - E_o^{3/2}] \right] $$

$$ T_R = 1.483 \times 10^7 \, m^{-1/2} \, F E_o^{-1/2} \, \exp \left[ - \beta E_o^{3/2} \right] $$

with

$$ \beta = 6.826 \times 10^7 \, m^{1/2} \, F^{-1} $$

If we consider a trap density $N(z_p, E_o)$, the resonant tunneling process will be an individual one if the density $N(z_p, E_o)$ is not too large. In what follows the criterion for independence of the interaction of the individual impurity atoms with the tunneling electron is defined. Let us consider two impurity atoms located at $r = 0$ and $r = R$ and represented by the potentials $V_1(r)$ and $V_2(r)$. The wave functions of the isolated traps are $\varphi_1(r)$ and $\varphi_2(r)$. The wave functions of the two centres can be written as a linear combination of $\varphi_1(r)$ and $\varphi_2(r)$ [20]:

If the electric field in the barrier is large enough the difference between the trap energy levels is also large. Its order of magnitude is $\Delta' \approx F \cdot R$ and we then have:

$$ \varphi_{12}(r) = \varphi_1(r) + \frac{W}{FR} \varphi_2(r) $$

where

$$ W = \langle \varphi_1 \mid V_1 \mid \varphi_2 \rangle - \langle \varphi_1 \mid \varphi_2 \rangle \langle \varphi_1 \mid V_2 \mid \varphi_1 \rangle $$

For two $\delta$ function potentials:

$$ W = \hbar (2 E_o/m)^{1/2} \, R^{-1} \, \exp(- \hbar^{-1}(2 m E_o^{3/2}) R). $$

(15)

Under these conditions the single trap level shift due to the presence of the second one is given by:

$$ \Delta E \approx \frac{2 W}{FR} E_o \langle \varphi_1 \mid \varphi_2 \rangle = (2 m^{-1/3} \, F^{-2/3} \, E_o^{3/2}) \times $$

$$ \times R^{-2} \times \exp[- 2 \hbar^{-1}(2 m E_o^{1/2} R)]. $$

(16)

This shift measures the amplitude of the interaction between two impurities. As a consequence the resonant tunneling transitions corresponding to many traps are independent if

$$ \Delta E < F. $$

In the case of a Schottky barrier one must have:

$$ R^{-2} \exp[- 2 \hbar^{-1}(2 m E_o^{1/2} R)] \times F^{-2} $$

$$ = 0.125 \, E_o^{-2} \, \exp(- \beta E_o^{3/2}) $$

(17)

i.e. approximately

$$ N(z_p, E_o) \lesssim (F/E_o)^3. $$

(18)

In this case the current that goes through the barrier is:

$$ J = \sum_{E_0} \int N(z_p, E_o) f(E_o, z_j) \, dz_j. $$

(19)

The function $f(E_o, z_j)$ shows a maximum for $E_o$ and $z_j$. If the trap density is assumed to be constant two cases should be considered:

i) The traps are quasi-continuously distributed in the semiconductor bandgap. The double maximum being very sharp the resonant tunneling current is essentially due to the traps in $E_{o_{\text{om}}}, z_m$. Eq. (19) becomes:

$$ J = n(E_{o_{\text{om}}}) f(E_{o_{\text{om}}}, z_m). $$

(20)

where $n(E_{o_{\text{om}}})$ stands for the surface density of traps at $E_{o_{\text{om}}}$. The detailed form of (20) is given by eq. (18) in [9].
Nevertheless the most frequently encountered case corresponds to a discrete distribution of energy levels. The current is then given by:

\[ J = \sum_{E_0} n(E_0') f(E_0', z_m(E_0')) \] (21)

where \( z_m(E_0') \) is the optimal coordinate for traps of energy \( E_0' \).

The prefactor in (13) varying slowly with \( z_j \) when compared to the exponential, \( z_m(E_0') \) can be easily computed by equating the arguments of the exponentials in (13) and (13'). This gives

\[ z_m(E_0') = (2^{2/3} - 1) E_0' F^{-1}. \] (22)

The variation of \( z_m(E_0') \) with the applied voltage is such that the energy level where the current passes through is constant and given by:

\[ E_0 = \phi_{BN} - 2^{2/3} E_0' \]

where \( E_0 \) is defined in figure 1.

The expression for the current going through the barrier is:

\[ J = 310^{-12} F m^{-1/2} \sum_{E_0} n(E_0') E_0^{-1/2} \times \exp - \beta E_0' N^2 [f(E_0') - f(E_0' + V)] \] (23)

when \( n(E_0') \) is expressed in cm\(^{-2}\).

Of course relation (23) is not valid beyond

\[ V = V_{BI} = 2^{2/3} E_0' \]

where \( V_{BI} \) represents the semiconductor built in voltage, i.e. the voltage at which the trap is level with the semiconductor conduction band. Another restriction arises at low temperature. In this case no carriers are present in the metal at \( E_0 \) if \( E_0 \) is higher than the metal fermi level. The current maximum then occurs at an energy level close to this fermi level and is given by:

\[ J = 2.3 \times 10^{-12} F m^{-1/2} \sum_{E_0} n(E_0') [\phi_{BN}^{1/2} - E_0'^{1/2}] \times \exp - \beta (\phi_{BN}^{3/2} - E_0'^{3/2}) + E_0'^{1/2} \exp \beta E_0'^{3/2})^{-1}. \] (24)

In order to estimate the amplitude of the resonant tunneling current we shall compare it to the direct tunneling one. This comparison will be carried out in a reversely biased AsGa Schottky barrier defined by the following magnitude:

\[ \phi_{BN} = 1 \text{ eV}, \quad N_D = 6.5 \times 10^{17} \text{ cm}^{-2}, \quad T = 300 \text{ K}, \quad m = 0.07 \varepsilon = 13.5. \]

The direct tunneling current \( J_D \) is calculated according to [11].

Figure 2 compares both contributions and clearly shows the amplitude of the resonant tunneling contribution. In this figure \( N_{TO} \) stands for the surface density necessary to equate the two contributions. The resonant tunneling current still enhances its amplitude at low temperature \( (T = 77 \text{ K}) \). The range of \( N_{TO} \) being \( 10^{1}-10^{9} \text{ cm}^{-2} \); these numbers were obtained for the same doping and biasing conditions as in figure 2.

These results are not in agreement with those obtained by (8) who predicted resonant currents of amplitudes \( 10^{11} \) times larger than direct tunneling current at low temperature.

Furthermore the minimum in the curves of figure 2 shows the competition existing between the direct and the resonant tunnel currents. Indeed, the growth of the resonant component is given by:

\[ S_{TR} = \frac{\partial \ln J}{\partial V} = \frac{q N_D}{eF^2} (1 + \beta E_0^{13/2}). \] (25)

Whereas the growth of the direct component is given by [11]:

\[ S_D = \frac{\partial \ln J_D}{\partial V} = \left( \frac{1}{kT} - \frac{\text{th} (E_{00}/kT)}{E_{00}} \right) \times \left( 1 + \text{th}^2 (E_{00}/kT) \right)^{-1}. \] (26)
where
\[ E_{00} = (N_D/4 \cdot m h^2)^{1/2} \]
and consequently does not depend on the reverse applied bias.

Under the bias threshold for which \( S_{TR} = S_D \) the resonant component increases at a rate larger than the direct one; above this threshold the contrary is true.

The slope of the curves \( N_T(V) \) is:

\[ \frac{\partial N_{T0}}{\partial V} = \frac{N_T J_D}{J} (S_D - S_{TR}) \quad (27) \]

this shows that the minimum in \( N_{T0}(V) \) occurs for voltages such that \( S_D = S_{TR} \). Although the linear approximation of the potential barrier would not be suitable for the forward biased regime the results obtained at \( V = 0 \) allow us to predict that even at low forward voltages the resonant current will make up a high proportion of the total current flowing through the barrier.

References

[19] When determining \( T(E, k) \) two approximations were made: i) we consider the barrier surface to be large enough to have
\[ \int e^{i(k-q')} d^2 q = (2\pi)^2 \delta(q-q') \]
ii) when relation (5) was integrated over \( q \) the argument of the exponential in (5') was developed to the first order up to \( q^2 \). This is possible because the exponential exhibits a sharp maximum for \( q = 0 \). Forthmore, an interference term connecting the direct to the resonant channel has been neglected.