Evaluation of the tunnelling current assisted by deep traps in schottky barriers

Grard Sarabayrouse, J. Buxo, A. Myszkowski, Daniel Esteve

► To cite this version:

Grard Sarabayrouse, J. Buxo, A. Myszkowski, Daniel Esteve. Evaluation of the tunnelling current assisted by deep traps in schottky barriers. *Revue de Physique Applique*, 1977, 12 (2), pp.433-437. 10.1051/rphysap:01977001202043300 . jpa-00244193

HAL Id: jpa-00244193

<https://hal.science/jpa-00244193>

Submitted on 1 Jan 1977

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destine au dpt et la diffusion de documents scientifiques de niveau recherche, publis ou non, manant des tablissements d'enseignement et de recherche franais ou trangers, des laboratoires publics ou privs.

Classification
Physics Abstracts
8.340

EVALUATION OF THE TUNNELLING CURRENT ASSISTED BY DEEP TRAPS IN SCHOTTKY BARRIERS

G. SARRABAYROUSE, J. BUXO, A. MYSZKOWSKI and D. ESTEVE

Laboratoire d'Automatique et d'Analyse des Systèmes du C. N. R. S.
7, avenue du Colonel Roche, 31400 Toulouse, France

(Reçu le 8 mars 1976, révisé le 14 juin 1976, accepté le 4 novembre 1976)

Résumé. — En s'appuyant sur les travaux de I. Lundström et C. Swensson relatifs au calcul des sections efficaces de capture par effet tunnel des pièges profonds, les auteurs proposent une première évaluation théorique de l'importance de la composante de courant tunnel assisté par la présence de pièges profonds dans les diodes Schottky.

Abstract. — Using the results of I. Lundström and C. Swensson for the tunneling capture cross-section of deep traps, the authors present a theoretical approach for accurately evaluating the tunneling current assisted by deep traps in Schottky diodes.

1. Introduction. — The tunneling current going through barriers containing deep traps has been discussed by several authors, among them : J. C. Penley [1], F. W. Schmidlin [2], G. H. Parker and C. A. Mead [3, 4], R. Combescot [5] and more recently by A. V. Chaplik and M. V. Entin [6]. One interesting feature of the $J(V)$ curves was already revealed by the analysis of G. H. Parker and C. A. Mead. Indeed their formalism accounts for the slope of the $J(V)$ curves that was experimentally observed at 77 K. The description given in detail here is aimed to provide an analytical expression of the trap assisted tunneling current that contains no adjustable parameters. In the first section the physical formalism is described, the second one presents its application to the case of a Schottky barrier. The comparison between this assisted current and the direct tunneling current is carried out.

2. The physical formalism. — A potential barrier $U(z)$ between a metal and a semiconductor including a deep trap at distance W from the metal and at energy E_L with respect to the bottom of the conduction band in the metal will be considered.

FIG. 1. — Energy diagram for the studied tunnel process.

In the WKB approximation an electron coming from the metal has the following wave function for $z > 0$, i. e. in the barrier :

$$\psi(r) = 2^{1/2} L^{-3/2} k_z (H_1^2(0) + k_z^2)^{-1/2} \exp(ik_x x + ik_y y) \exp\left(-\int_0^z H_1(t) dt\right) \quad (1)$$

where L^3 is the volume of the metal,

$$k_x^2 + k_y^2 + k_z^2 = 2 m_1 \hbar^{-2} E_L,$$

$$H^2(z) = 2 m_r \hbar^{-2} (U(z) - E_L), \text{ and } H_1^2(t) = H^2(t) + k_x^2 + k_y^2.$$

m_1 and m_r are the effective masses of an electron respectively in the metal and in the semiconductor.

The wave function of an electron bound to the trap represented by a Dirac delta function [7] is taken to be :

$$\psi_r(r) = (2\pi)^{-1/2} H^{1/2}(W) r^{-1} \exp(-H(W)r). \quad (2)$$

Following J. Bardeen [8] and I. Lundström *et al.* [9] the transition probability between the metal and the trap is (see appendix) :

$$P_{mp} = 2\pi\hbar^{-1} |T_{r1}|^2 \frac{\partial n}{\partial E} \quad (3)$$

with the tunneling transition matrix element :

$$T_{r1} = \int \psi_r(r) (H - E_L) \psi_1(r) d^3r \quad (4)$$

and with the density of states :

$$\frac{\partial n}{\partial E} = \left(\frac{L}{2\pi}\right)^3 \frac{4m_1}{\hbar^2 k_z} d^2k_p \quad (5)$$

corresponding to the E_L energy level and to a given value of k_p .

Finally, one obtains for the probability P_{mp} :

$$P_{mp} = \frac{8\hbar m_1}{m_r^2} \int_0^{k_0} \frac{H(W)k_z}{H^2(0) + k_0^2} \exp\left[-2 \int_0^W (H^2(t) + k_p^2)^{1/2} dt\right] k_p dk_p \quad (6)$$

where

$$k_0^2 = 2m_1\hbar^{-2}E_L = k_p^2 + k_z^2.$$

The wave function of an electron coming from the semiconductor is :

$$\psi_1(r) = L^{-3/2} k_z^{1/2} H^{-1/2}(z) \exp(ik_x x + ik_y y) \exp\left(-\int_z^a H_1(t) dt\right), z < a \quad (7)$$

where a is the classical turning point.

The electron transition probability between the trap and the semiconductor can be obtained by the previous method leading to :

$$P_{sep} = \hbar m_r^{-1} H(W) \int_0^{k_0} (H^2(W) + k_p^2)^{-1/2} \exp\left[-2 \int_W^a (H^2(t) + k_p^2)^{1/2} dt\right] k_p dk_p \quad (8)$$

where

$$k_0'^2 = 2m_r\hbar^{-2}(E_L - E_C),$$

and E_C is the energy of the bottom of the semiconductor conduction band.

The detailed balance principle will now be applied in order to compute the current density carried through the trap between the metal and the semiconductor.

The current density components for the two elementary transitions can then be written in the form

$$\begin{aligned} j_{mp} &= j_1 - j_2 = qN_t P_{mp}(f_m - f_t) \\ j_{psc} &= j_3 - j_4 = qN_t P_{sep}(f_t - f_{sc}) \end{aligned} \quad (9)$$

where N_t is the density of traps and f_m, f_{sc}, f_t stand for the occupancy factors in respectively the metal, the semiconductor and the trap at energy E_L .

In the steady state situation the equality between these two currents allows one to determine the trap occupancy f_t . The tunneling current at E_L then is :

$$j = qN_t P(f_m - f_{sc}) \quad (10)$$

with

$$P^{-1} = P_{mp}^{-1} + P_{sep}^{-1}.$$

3. **Application to the case of a Schottky barrier.** — When expressions (6) and (8) are integrated ⁽¹⁾ in the case of a parabolic barrier

$$U(z) = + q^2 \frac{N_D(d-x)^2}{2\varepsilon} - q^2 \frac{N_D d^2}{2\varepsilon} + q\varphi_{BN} + q\varphi_{FM} \text{ (see Fig. 1) ,}$$

one obtains :

$$P_{mp} = \frac{4 \hbar m_1}{m_r^2} \frac{H(W) k_0/A}{(H^2(0) + k_0^2)} \{ 1 - (Ak_0^2)^{-1/2} D((Ak_0^2)^{1/2}) \} \exp - 2 F \quad (11)$$

$$P_{scp} = \pi^{1/2} \hbar m_r^{-1} H(W)^{-1/2} A_1 \exp(A_1 H^2(W)) \{ \varphi(A_1^{1/2}(k_0 + H^2(W))^{1/2}) - (A_1^{1/2} H(W)) \} \exp - 2 F_1 \quad (12)$$

with :

$$\begin{aligned} A &= \xi(d, d-W) = C^{-1/2} \ln[\eta C^{1/2} + (C\eta^2 + R)^{1/2}]_{\eta=d-W}^{\eta=d} \\ F &= \chi(d, d-W) = \frac{1}{2} R \xi(d, d-W) + \left[\frac{1}{2} \eta (C\eta^2 + R)^{1/2} \right]_{\eta=d-W}^{\eta=d} \\ A_1 &= \xi(d-W, d-a) \quad F_1 = \chi(d-W, d-a) \\ C &= q^2 N_D m_r \varepsilon^{-1} \hbar^{-2} \quad D = + 2 m_r \hbar^{-2} (U(d) - E_L) \end{aligned}$$

where N_D is the doping level in the semiconductor, d the space charge width, φ_{BN} the barrier height and φ_{FM} the energy of the Fermi level in the metal with respect to the bottom of the metal conduction band.

The most important physical features of the current corresponding to the Schottky barrier case can be made clearer using the triangular barrier approximation

$$U(z) = - \frac{q^2 N_D dz}{\varepsilon} + q\varphi_{BN} + q\varphi_{FM} ,$$

one then obtains by using Boltzmann statistics :

$$j = 2^{-1/2} q^3 N_D N_T d\varepsilon^{-1} m_r^{-1/2} F(E_L, W) \cdot G(E_L, W) (1 - e^{qV/kT}) \quad (13)$$

with

$$F(E_L, W) = \exp\{ - \lambda(U(W) - E_L)^{3/2} - E_L/kT \} (U(W) - E_L)^{-1/2} \quad (14)$$

$$G^{-1}(E_L, W) = \{ 1 + 4 m_r^{1/2} m_l^{-1/2} (m_r m_l^{-1} \theta + E_L) (\theta^{1/2} - \Omega^{1/2}) \Omega^{-1} E_L^{-1/2} \exp - \lambda(\theta^{3/2} - 2 \Omega^{3/2}) \} \quad (15)$$

and

$$\lambda = \frac{4}{3} (2 m_r \hbar^{-2})^{1/2} , \quad \varepsilon q^{-2} N_D^{-1} d^{-1} , \quad \theta = U(0) - E_L , \quad \Omega = U(W) - E_L .$$

It appears that j presents a double maximum value depending on both E_L and W . This is due to the fact that, on the one hand, P grows with the increasing values of E_L whereas both f_m and f_{sc} decrease ; the value of E_L corresponding to this maximum is called E_M . On the other hand j passes through another maximum for the particular value W_M where $P_{mp} = P_{scp}$.

The expressions (15) and (14) respectively allow one to calculate E_M and W_M . The expressions :

$$E_M = [2^{2/3} U(W) - U(0)] (2^{2/3} - 1)^{-1} \quad (16)$$

$$W_M = 2^{-5/3} (2^{2/3} - 1) \hbar^2 q^2 N_D d m_r^{-1} (kT)^{-2} \quad (17)$$

provide good approximations for these two values. The current at this maximum is then given by :

$$j = 2^{1/3} q N_t \hbar^{-1} kT (1 - e^{qV/kT}) e^{-\frac{q\varphi_{BN}}{kT}} \exp \left[\frac{1}{6} (\hbar q^2 N_D d m_r^{-1/2} \varepsilon^{-1} (kT)^{-3/2})^2 \right] . \quad (18)$$

⁽¹⁾ The exponential is a rapidly decreasing function of k_p and only the first two terms in the development of its argument will be considered.

This current is compared to the direct tunneling current J_T , also going through the barrier [10], on figure 2. This figure directly provides on the y-axis the value of the trap density N_t , for which j equals J_T

FIG. 2. — Comparison between the trap assisted tunneling current and the direct tunneling current (in the range where Boltzman statistics applies).

and corresponds to the case of a reversely biased metal-silicon Schottky barrier at room temperature for which the value $\phi_{BN} = 0.6$ eV has been assumed. The values of W_M given by (17) appear then to be comprised in the following ranges : $5 \text{ \AA} < W_M < 100 \text{ \AA}$ for $10^{17} \text{ cm}^{-3} < N_D < 5 \times 10^{17} \text{ cm}^{-3}$ and $0 < V < 10 \text{ V}$.

This result shows that the occurrence of this trap assisted current in a reversely biased Schottky barrier is far from being unlikely. Indeed, recent backscattering measurements carried out by A. Martinez [11] show that, after standard stabilizing annealing treatments, a large density of metallic centres can be present over distances as large as $500 \text{ \AA}$ of the metallic interface.

The present theory can then account for the large values of the reverse currents in these barriers that have not been clearly explained up to now.

Appendix. — It will be now shown that Bardeen's method [8] can be applied to calculate either P_{mp} or P_{scp} .

The trap is assumed to be well described by a short range potentiel V_p containing a simple bound state ; as we are here neglecting the direct tunneling

current we shall assume that ψ_1 only contains its decreasing component. If the trap is located far away enough from the boundary, the overlap between ψ_1 and ψ_r is small and the total wave function of the fundamental state of the system is well approximated by :

$$\psi(r, t) = a(t) \psi_1(r) \exp\left(-\frac{iE_1 t}{\hbar}\right) + b(t) \psi_r(r) \exp\left(-\frac{iE_r t}{\hbar}\right) \quad (\text{A.1})$$

where E_1 and E_r are respectively the energies corresponding to ψ_1 and ψ_r . It is now assumed that at time $t = 0$ the electron is in the state ψ_1 so that $a(0) = 1$ and $b(0) = 0$. The Schrodinger equation integrated over the barrier volume V with $\psi_r(r)$ or $\psi_1(r)$ leads to :

$$\frac{db}{dt} = \frac{1}{i\hbar} \exp\left[\frac{it}{\hbar}(E_r - E_1)\right] T_{r1} \quad (\text{A.2})$$

with

$$T_{r1} = \int_V \psi_r(r) (H_0 + V_p - E_1) \psi_1(r) d^3r. \quad (\text{A.3})$$

It is assumed that for a trap inside the barrier :

$$\int_V |\psi_r|^2 d^3r \approx 1. \quad (\text{A.4})$$

The integration over the time variable in (A.2) allows one to obtain $b(t)$. The current corresponding to the wave function (A. 1) is then given by :

$$j = \hbar m^{-1} T_{r1} (E_r - E_1)^{-1} \sin[t(E_r - E_1)/\hbar] \times [\psi_r \nabla \psi_1 - \psi_1 \nabla \psi_r]. \quad (\text{A.5})$$

In order to obtain the transition probability we integrate this current over the surface of the boundary. (As the barrier volume is very large this integral can be transformed in an integral over the barrier volume with the help of the Gauss theorem.) This leads to :

$$J = \frac{2}{\hbar} |T_{r1}|^2 (E_r - E_1)^{-1} \sin[t(E_r - E_1)/\hbar]. \quad (\text{A.6})$$

The averaged probability is then given by :

$$P = \lim_{t \rightarrow \infty} t^{-1} \int_0^t |J| dt = \frac{2\pi}{\hbar} |T_{r1}|^2 \cdot \delta(E_r - E_1).$$

This formula has been used by I. Lundström and C. Swensson [9]. As we do not use here particular forms of ψ_r and ψ_1 it remains valid for any barrier and any short range trap potential if the trap is located sufficiently far away from the barrier boundary. This condition is satisfied in almost all the situations of the problem treated here.

References

- [1] PENLEY, J. C., *Phys. Rev.* **128** (1962).
 - [2] SCHMIDLIN, F. W., *J. Appl. Phys.* **37** (1966).
 - [3] PARKER, G. H. and MEAD, C. A., *Appl. Phys. Lett.* **14** (1969) 21.
 - [4] PARKER, G. H. and MEAD, C. A., *Phys. Rev.* **184** (1969) 780.
 - [5] COMBESCOT, R., *J. Phys. C.*, **4** (1971) 2611.
 - [6] CHAPLIK, A. V. and ENTIN, M. V., *Sov. Phys. JETP* **40** (1974) 106.
 - [7] LUCOWSKY, G., *Solid State Commun.* **3** (1965) 299.
 - [8] BARDEEN, J., *Phys. Rev. Lett.* **6** (1961) 57.
 - [9] LUNDSTRÖM, I. and SWENSSON, C., *J. Appl. Phys.* **43** (1972) 5045.
 - [10] PADOVANI, F. A. and STRATTON, R., *Solid State Elect.* **9** (1966) 695.
 - [11] MARTINEZ, A., Thesis, P. Sabatier University Toulouse, n° 704 (1976).
-