Electron tunneling through thin insulating films*

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It is shown by means of an exactly solvable one-dimensional model for a symmetric metal-insulator-metal structure, that the heuristic method [based on a modified WKB (MWKB) approximation] recently proposed by Kurtin, McGill, and Mead to determine the dispersion relation E-k' within the gap of the insulator from empirical data of tunneling current, gives reliable results. The reason is that the MWKB method reproduces the exact tunneling probability in order of magnitude for all energies in the gap. It is also shown that the usual WKB method applied to the trapezoidal model underestimates the tunneling probability by orders of magnitude.

INTRODUCTION

Recently Kurtin, McGill, and Mead[1] have proposed a new analytical technique for determining the energy-momentum dispersion relation E-k' within the forbidden gap of a solid, and they succeeded in understanding quantitatively the tunneling current observed in GaSe in terms of this E-k' relation. The technique is based on the calculation of the tunneling probability T using the WKB approximation[2] with the attenuation factor κ replaced by the complex wave vector k' within the gap of the insulator. The theoretical foundation for applying this procedure, which hereinafter we call the modified WKB (MWKB) method, remained however on a heuristic basis.

Here, we study an exactly solvable one-dimensional model for the electron tunneling in a symmetric metal-insulator-metal (MIM) structure which allows us to test the adequacy of the MWKB method by comparison of the exact and approximate transmission probabilities through the insulator. We conclude that although the MWKB method reproduces the exact T only in order of magnitude, it can be considered a rather good approximation from the point of view of determining the E-k' relation from empirical data of the tunneling current.

MODEL

The insulating thin film is described by a finite succession of δ-function-type potentials equally spaced, which if continued indefinitely gives rise to a band structure simulating that of the bulk insulator. The distance between the δ functions, a, represents the lattice constant of the insulator and Na its width, where N is the number of δ's (Fig. 1). The metal is described by a constant potential whose zero coincides with that of the insulator; thus we avoid unnecessary complications with the matching of the wave functions at the interfaces whose only effect is to give rise to reflections that are irrelevant to our problem.[3] If the zeros do not coincide, this introduces only a preexponential factor in the transmission probability.

Finally, the potential describing the MIM structure is

$$V(x) = \sum_{n=1}^{N} aV_0\delta(x - na) \quad , \tag{1}$$

where V_0 is a parameter which measures the strength of the potential.

TRANSMISSION PROBABILITY

A. Exact solution

A solution of the Schrödinger equation in the interval $na < x < (n+1)a$ can be written in the form

$$\psi_n(x) = A_n\, e^{ikx} + B_n\, e^{-ikx} \tag{2}$$

with $k = (2mE/\hbar^2)^{1/2}$, where m is the electron mass and E the electron energy. A_n and B_n are integration constants to be determined in such a way that

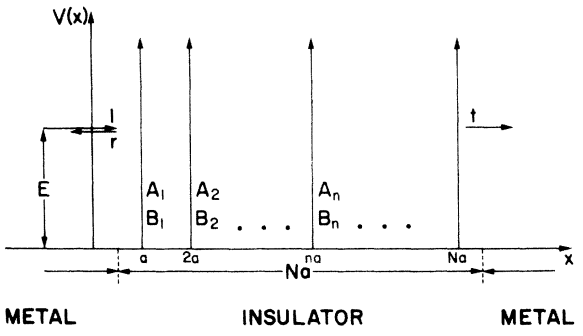

FIG. 1. Model potential for a symmetric MIM structure. The vertical arrows denote equally spaced δ-type potentials. The horizontal arrows denote an incoming electron from the left metal with energy E and amplitude 1 which is reflected with amplitude r and transmitted through the insulator with amplitude t. A_n and B_n are the amplitudes of the forward and backward plane waves, respectively, in the interval n.

the wave function $\psi(x)$ is continuous everywhere and such that[4]

$$\psi_n'(na) - \psi_{n-1}'(na) = \lambda\psi_n(na) \tag{3}$$

for $n = 1, \ldots, N$, where $\psi_n'(x)$ denotes the derivative of $\psi_n(x)$ with respect to x and $\lambda = 2maV_0/\hbar^2$. We are interested in the boundary conditions $A_0 = 1$, $B_0 = r$, $A_N = t$, and $B_N = 0$ corresponding to an incident plane wave coming from the left metal with unit amplitude which is reflected with amplitude r and transmitted through the film with amplitude t.

The recurrence relation between the integration constants in two subsequent intervals can be written in the matrix form[5]

$$\begin{pmatrix}\alpha_n\\ \beta_n\end{pmatrix} = P\begin{pmatrix}\alpha_{n-1}\\ \beta_{n-1}\end{pmatrix}, \tag{4}$$

where

$$\alpha_n = A_n\, e^{ikna}, \quad \beta_n = B_n\, e^{-ikna}, \tag{5}$$

and

$$P = \begin{pmatrix}(1-\lambda i/2k)e^{ika} & -(\lambda i/2k)e^{-ika}\\ (\lambda i/2k)e^{ika} & (1+\lambda i/2k)e^{-ika}\end{pmatrix}. \tag{6}$$

Hence, for a succession of N δ functions, we have

$$\begin{pmatrix}\alpha_N\\ \beta_N\end{pmatrix} = P^N\begin{pmatrix}\alpha_0\\ \beta_0\end{pmatrix}, \tag{7}$$

that is,

$$\begin{pmatrix}te^{ikNa}\\ 0\end{pmatrix} = P^N\begin{pmatrix}1\\ r\end{pmatrix}, \tag{8}$$

which leads to the transmission probability

$$T = |t|^2 = 1/|(P^N)_{22}|^2, \tag{9}$$

where $(P^N)_{hj}$ is the (h,j) element of the matrix P to the Nth power.

B. MWKB approximation

When the succession of δ functions is extended indefinitely ($N \to \infty$), the resulting periodic potential gives rise to the band structure of the bulk insulator (Fig. 2). The electron dispersion relation E-k' within a forbidden energy region is given by[6]

$$\left|\frac{\lambda a}{2}\frac{\sin ka}{ka} + \cos ka\right| = \cosh k'a. \tag{10}$$

In the MWKB approximation, the transmission probability becomes

$$T_{\mathrm{MWKB}} = e^{-2Nk'a}. \tag{11}$$

ANALYTICAL RELATIONSHIP BETWEEN T AND T_{MWKB}

Let

$$R = \begin{pmatrix}r_{11} & r_{12}\\ r_{21} & r_{22}\end{pmatrix} \tag{12}$$

be the matrix that diagonalizes P, that is,

$$p = RPR^{-1} = \begin{pmatrix}p_- & 0\\ 0 & p_+\end{pmatrix}, \tag{13}$$

where the eigenvalues of P can be written in the form

$$p_+ = e^{k'a}, \quad p_- = e^{-k'a}, \tag{14}$$

with k' given by Eq. (10).[5]

If R diagonalizes P, then it also diagonalizes any power of P

$$p^N = RP^NR^{-1} = \begin{pmatrix}p_-^N & 0\\ 0 & p_+^N\end{pmatrix} \tag{15}$$

or

$$P^N = R^{-1}\, p^N\, R, \tag{16}$$

and from this equation we obtain

$$(P^N)_{22} = P_+^N\,\frac{1-(p_-/p_+)^N\mu}{1-\mu}, \tag{17}$$

with $\mu = r_{12}r_{21}/r_{11}r_{22}$. From the case $N = 1$ we have

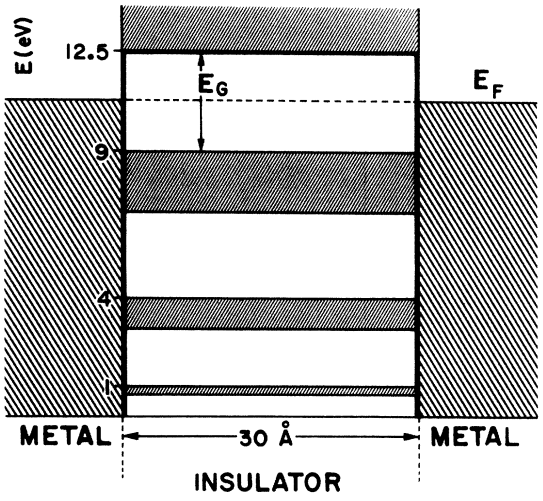

FIG. 2. Energy-band relations at the metal-insulator-metal interfaces with no bias applied. The band structure of the insulator, calculated with the parameters given in the text, is indicated with the dashed regions corresponding to allowed energy bands. E_F is the Fermi energy of the metal and E_G is the energy gap of the insulator. The heavy line represents the square potential barrier used in the trapezoidal model.

$$\mu = \frac{P_{22} - p_+}{P_{22} - p_-} , \tag{18}$$

and from Eqs. (9), (11), and (17) we obtain the following analytical relation between the exact and approximate transmission probabilities through N δ's:

$$\frac{T_{\mathrm{MWKB}}}{T} = \left| \frac{1 - (p_-/p_+)^N \mu}{1 - \mu} \right|^2 . \tag{19}$$

Not very near the edges of the forbidden energy regions $p_+ \gg p_-$ and we can write

$$T \approx T_{\mathrm{MWKB}} |1 - \mu|^2 . \tag{20}$$

NUMERICAL RESULTS

The band structure calculated from Eq. (10) using the values $a = 6.12$ Å and $V_0 = 8$ eV (to give $\hbar^2\pi^2/2ma^2 = 1$ eV and $\lambda a = 8\pi$) is shown in Fig. 2.

The transmission probabilities T and T_{MWKB} were calculated from Eqs. (9) and (11), respectively, for the case of five δ functions and for energies within the forbidden energy region 9.0–12.5 eV. These values were chosen to correspond with a typical insulating film of 30-Å width and an energy gap of 3.5 eV. The results are shown in Fig. 3. The E-k' characteristics obtained from Eq. (10) for the same gap are given in Fig. 4.

We have also calculated the transmission probability T_{WKB} given by the "trapezoidal model"[1,7,8] in the usual WKB approximation. This model, commonly used to describe the work functions at interfaces with insulators, considers the forbidden gap of the insulator as a simple potential barrier. In our case, for a square potential as shown in Fig. 2, we have[2]

$$T_{\mathrm{WKB}} = e^{-10\kappa a} \tag{21}$$

with

$$\kappa a = \pi(12.5 - E)^{1/2} \tag{22}$$

where E is in eV (Fig. 3). For comparison with the dispersion relation used in the MWKB method, the relation (22) has also been plotted in Fig. 4.

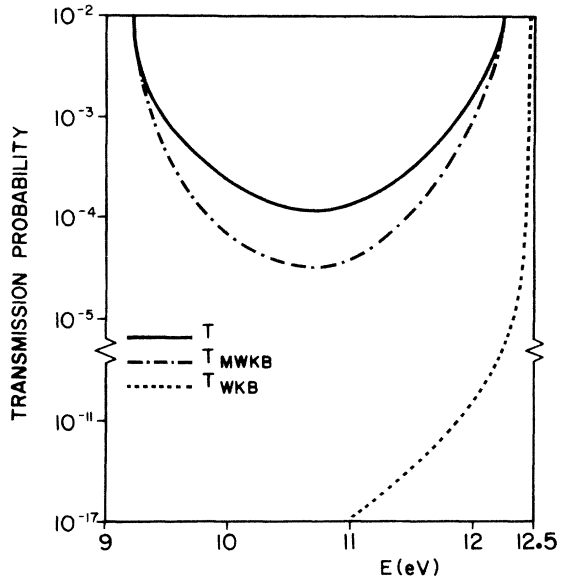

FIG. 3. Transmission probabilities calculated with the parameters indicated in the text. T: full line; T_{MWKB}: dashed line; T_{WKB}: point line. (Notice the change of scale in ordinates.)

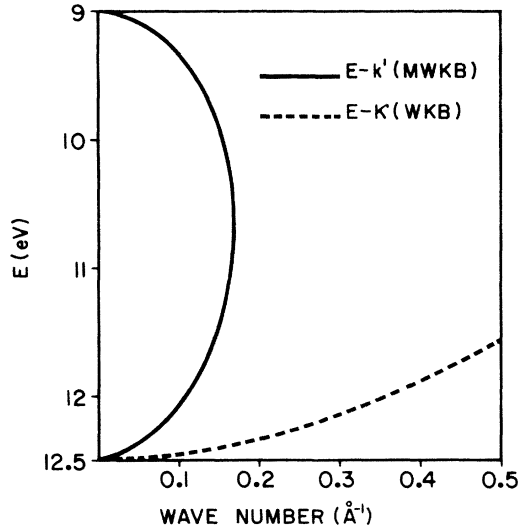

FIG. 4. Dispersion relation within the energy gap. E-k' characteristics of the insulator from band structure, Eq. (10): full line; E-κ relation from usual WKB approximation, Eq. (22): dashed line.

DISCUSSION

The MWKB method reproduces the exact transmission probability T in order of magnitude for all energies in the gap (Fig. 3). In Eq. (20) the factor T_{MWKB} contributes overwhelmingly since, according to Eq. (11), it depends exponentially on the E-k' relation. The preexponential factor $|1 - \mu|^2$ is a slowly varying function of the energy of the order of 1. It is for this reason that the MWKB method is a rather good approximation to derive the E-k' relation of the insulator within the gap from the empirical T obtained by means of tunneling experiments.

From Eqs. (11) and (21) and the data of Fig. 4, it is apparent that T_{WKB} results are several orders of magnitude smaller than T_{MWKB}. For instance, for $N = 5$ and an energy 0.35 eV below the bottom of the conduction band, we obtain $T_{\mathrm{MWKB}} \cong 3.5 \times 10^{-3}$ and $T_{\mathrm{WKB}} \cong 10^{-8}$. That is, the usual WKB method applied to the trapezoidal model strongly underestimates the transmission probability (Fig. 3).

Since electron tunneling through an insulating film is essentially a one-dimensional problem, we think that the conclusions derived from our one-dimensional model would not be seriously modified when the three-dimensional nature of the actual processes involved in the tunneling are taken into account.

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[1]S. L. Kurtin, T. C. McGill, and C. A. Mead, Phys. Rev. B 3, 3368 (1971).

[2]Eugen Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970), Chap. 7.

[3]In the calculation of the tunneling current in Ref. 1, the factor describing these reflections, $g(E, k_{\parallel})$, is put equal to 1; that is, the reflections at the interfaces are neglected.

[4]Details about the mathematical treatment of δ-function-like potentials are given for instance in I. I. Gol'dman and V. D. Kirvchenkov, *Problems in Quantum Mechanics* (Pergamon, London, 1961), p. 9, problems 13, 14 and 15 and their solutions.

[5]Reference 2, Chap. 6.

[6]R. de L. Kronig and W. G. Penney, Proc. Roy Soc. A 130, 499 (1931).

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[8]John G. Simmons, J. Appl. Phys. 34, 1793 (1963).