Inelastic tunneling through optical barriers

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Tunneling of electrons through optical potential barriers gives rise to an increase in current density. This is due to the imaginary part of the complex potential, which absorbs more flux into the barrier and, as a result of a continuity equation, a larger current is transmitted. This is corroborated by experiments on metal-insulator-metal junctions.

Hitherto a number of theoretical attempts have been made to evaluate the tunneling current.[1–14] These include the approximation of the barrier by a series of square wells,[4–8] use of a mean barrier height,[13,14] parametrization of the effective mass m^* of the electron,[9,10] and the assumption of a low density of isolated traps in the barrier.[9] Caldeira and Leggett[11] have included the effect of dissipative forces in which friction plays an important role. In all these papers, only qualitative agreement with experiment has been obtained.

The purpose of the present paper is to make an interesting observation: An increase in tunneling current is possible if the barrier is represented by a complex potential. Introduction of a small negative imaginary part $W(r)$ in the potential term of the wave equation for the penetrating particle is shown to increase the current.[15] The optical potential theory is a well-established theory to treat the metastable (or quasistationary) states in which particles move "inside the system" for a considerable period of time. The quasidiscrete energy spectrum of these states will consist of a series of broadened levels, and the energy itself is a set of complex values:

$$E=E_0\pm i\,\Delta E\ .$$

The imaginary part of the potential introduces a real momentum inside the barrier which is used to evaluate the tunneling time and a value of 10^{-15} sec is obtained.[16] This is in agreement with the experimental value.

Let us for simplicity consider a rectangular barrier depicted in Fig. 1:

$$V(x)=\begin{cases}0, & x<0\\ V_0\pm iW_0, & 0<x<b\end{cases} \tag{1}$$

where b is the width of the barrier, V_0 is the height, and W_0 the corresponding imaginary part. In the three regions of interest, the solutions to the Schrödinger equations are[17]

$$\psi_1=e^{ik_1x}+Be^{-ik_1x}\ , \tag{2a}$$

$$\psi_2=Ce^{-k_2x\pm ik_3x}\ , \tag{2b}$$

$$\psi_3=De^{i(k_1+\Delta k)x}\ , \tag{2c}$$

where $k_1=\sqrt{E}$, and k_2 and k_3 are, respectively, the imaginary and real parts of the momentum inside the barrier. The momentum spread Δk due to the inelastic processes inside the barrier is very small:

$$k_2=R\cos(\alpha/2)\ , \tag{3a}$$

$$k_3=\mp R\sin(\alpha/2)\ , \tag{3b}$$

where

$$R=(V_0-E)^{1/2}\left[1+\frac{W_0^2}{(V_0-E)^2}\right]^{1/4}$$

and

$$\alpha=\tan^{-1}\left[\frac{W_0}{V_0-E}\right]\ .$$

Here we use the atomic units $\hbar=1$, $m=\frac{1}{2}$, $e^2=2$. The effect of an applied external voltage will be considered later.

It may be observed that Eq. (2b) is an approximate expression but valid for treatment of tunneling through thin films. The sign $\mp$ for k_3 corresponds to the sign $\pm$ of W_0. It can be easily shown[18] with the use of the perturbation theory that the energy spread $i\epsilon$, which is twice the width ΔE of the outcoming electron spectrum, is very much smaller since $|\psi_2^*\psi_2|\ll 1$.

$$i\epsilon=\tfrac{1}{2}i\,\Delta E=i\int\psi_2^*W_0\psi_2dx\ . \tag{4}$$

By matching the wave functions at $x=0$ and b, we get the transmission coefficient

$$D^*D=C^*Ce^{-2k_2b}\ , \tag{5a}$$

where

$$C=2ik_1/[-k_2+i(k_1+K_3)]\ . \tag{5b}$$

In region II the fluctuating part due to k_3 (see Fig. 1) is superimposed over the attenuating function $\exp(-2k_2x)$.

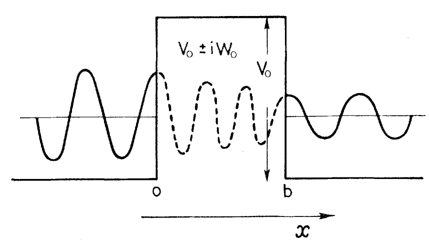

FIG. 1. Rectangular barrier with a complex potential. The wave function within the barrier is a decaying function with a superposition of an oscillator function.

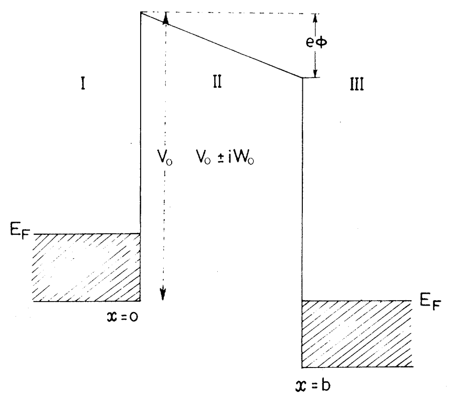

FIG. 2. Distorted barrier for the metal-insulator-metal junction when a potential $e\phi$ is applied across the insulator.

For reasons mentioned below only the negative sign for W_0 is meaningful. This proves that the imaginary part of the potential inside the barrier can augment the magnitude of the current. Physically we explain it as follows: The reflection coefficient B^*B (see Fig. 1) is given by

$$B^*B=\frac{k_2^2+(k_1-k_3)^2}{k_2^2+(k_1+k_3)^2} . \tag{6}$$

The imaginary potential absorbs more flux into the barrier and as a result of continuity equation, a larger current emerges at $x=b$. On the other hand, when the imaginary part is positive, k_3 is negative, resulting in the increase of B^*B. Also when $W_0=0$, $k_3=0$ and the tunneling current becomes equal to the usual elastic tunneling current.

Introduction of iW_0 in the potential changes the equation of continuity slightly. Using the wave equation for a particle moving through an optical potential and its complex conjugate, we get the following continuity equation:

$$\frac{\partial}{\partial t}(\psi^*\psi)=i\vec{\nabla}\cdot(\psi^*\vec{\nabla}\psi-\psi\vec{\nabla}\psi^*)\pm 2iW_0\psi^*\psi . \tag{7}$$

For a one-dimensional barrier this reduces to

$$\frac{\partial\rho}{\partial t}=i\vec{\nabla}_x\cdot\left(\psi^*\vec{\nabla}\psi-\psi\vec{\nabla}\psi^*\pm i2\int W_0\psi^*\psi\,dx\right)$$

$$=-\vec{\nabla}_x\cdot(J_1\pm iJ_2) . \tag{8}$$

The inelastic processes introduce an imaginary current J_2. We hasten to add that the effect of W_0 is in both J_1 and J_2 through the wave function ψ.

In the present problem, we get the current density J at $x\geq b$ from Eqs. (2)—(5) as

$$J=k_1(D^*D) , \tag{9}$$

where we have omitted Δk which is negligibly small compared to k_1.

It is obvious from Eq. (3) that as W_0 increases, α and k_3 increases. The barrier attenuating factor $\exp(-2k_2b)$ grows in magnitude and changes the flux. The situation, however, is entirely different when $E>V$. The imaginary part of the momentum in this case becomes k_3 and the real part is k_2. Then $\psi_2=C\exp[(ik_2-k_3)x]$, assuming W_0 to be negative. As $|W_0|$ increases, k_3 increases and the current density falls off. This is the usual flux absorption effect of W_0 that we come across in inelastic reactions.

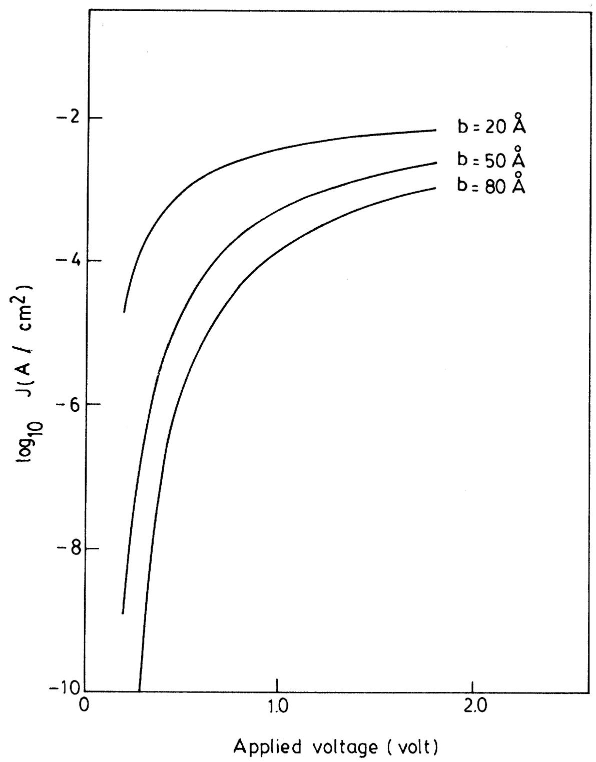

FIG. 3. Applied voltage vs the logarithm of the current density for Al_2O_3 films of thickness b.

We are now in a position to address the problem of tunneling of electrons through metal-insulator-metal junctions under an applied external field. Let us consider an oxide film of thickness b across which a voltage ϕ is applied. The barrier is distorted to assume a trapezoidal form as depicted in Fig. 2. The transmission coefficient T is calculated using the WKB approximation,[17,19]

$$T=\exp\left\{-\frac{4b}{3e\phi}\left[[(V_0-E)^2+W_0^2]^{3/4}\cos\left[\frac{3\beta}{2}\right]\right]\right\} , \tag{10}$$

with

$$\beta=\tan^{-1}\left[\frac{W_0}{V_0-E}\right] .$$

It is easily seen from the above equation that when $W_0\to 0$, the usual expression for the transmission coefficient T is recovered.[20] More realistic forms for the potential barriers could be used. Also a treatment using Airy functions[21] can be carried out to make a comprehensive study.

A typical calculation for Al-O-Al junction is carried out

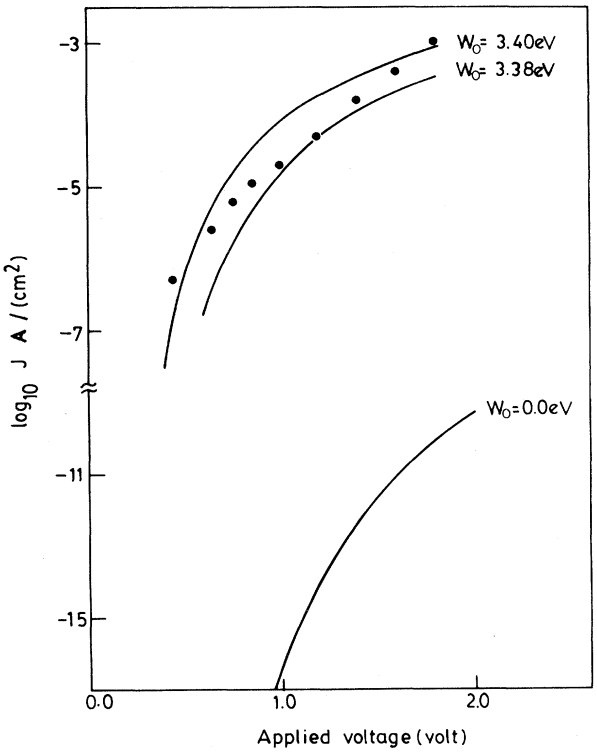

FIG. 4. Comparison of experimental values (dotted) of the tunneling current densities taken from Ref. 2 with calculated values for a thickness 80 Å of the oxide film.

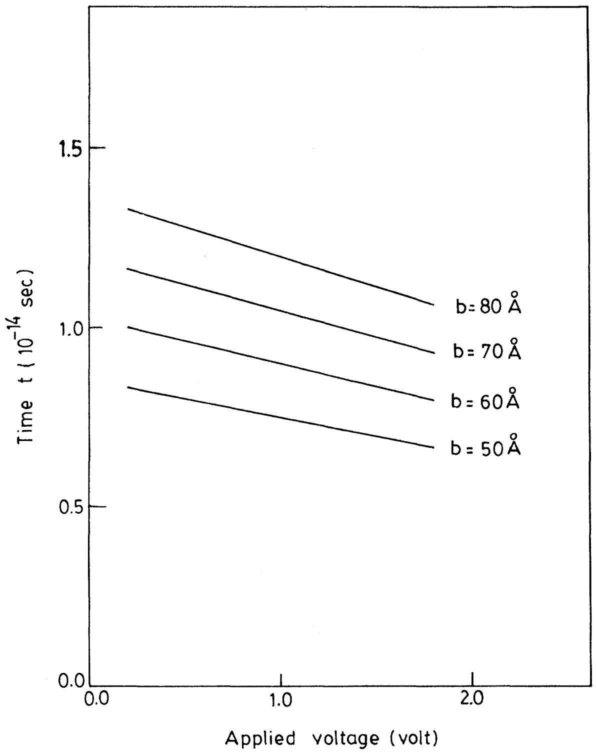

FIG. 5. Applied voltage vs tunneling time for different thicknesses (b) of the oxide film.

with the values of V_0 and E taken from Ref. 10. The values of W_0 are indicated in Figs. 3–5. It is usually around 2 eV which is just a fraction of the value of V_0. The agreement between the theoretical and experimental values is good.

In conclusion, we claim that a straightforward method of treating inelastic tunneling of electrons has been evolved. An important observation is made in the present study: An optical potential for barriers leads to a current density higher than the usual tunneling currents.

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