Some Properties of Exponentially Damped Wave Functions*

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We know from Bloch's theorem that the wave function ψ of an electron in a semiconducting or insulating crystal can be written

$$\psi = e^{ikx}u(x), \tag{1}$$

where k is the wave vector of the state and $u(x)$ is a periodic function with the lattice period of the crystal. Over reasonable distances the $u(x)$ part of the function averages out, and we can view the propagating part e^{ikx} as a quasi-particle behaving in much the same way as a particle in free space. The dynamics of this particle are given by the dispersion relation between the wave vector k and the energy E. For a semiconductor or insulator with a forbidden gap, the dispersion relation is something like the one shown in Fig. 1.

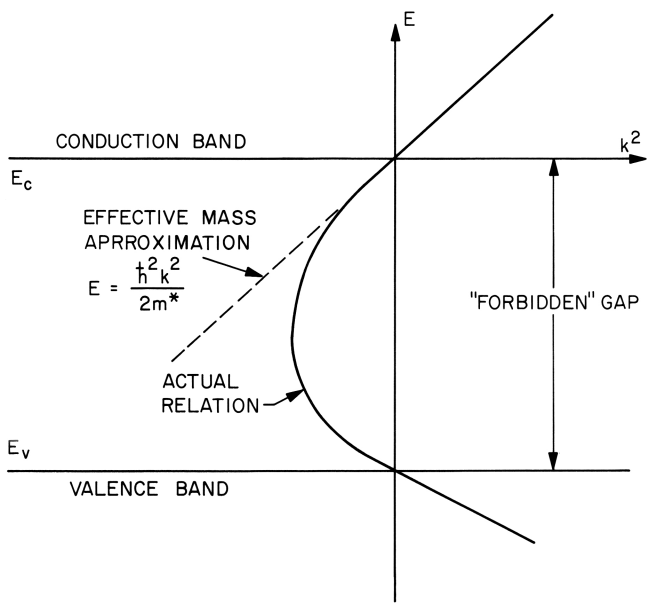

Figure 1: Energy-momentum relationship in a semiconductor or insulator.

Note that we have plotted E versus k^2 rather than the more conventional E versus k. The reason is as follows: It can be shown rather generally that near one of the band edges (E_c or E_v) the energy is quadratic in k, and is usually written $E = \hbar^2k^2/2m^*$ by analogy with the free electron. Here, m^* is the effective mass of the quasi-particle. This form is shown by the straight line in Fig. 1. For $E > E_c$ and

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$E < E_v, k^2$ is positive; therefore k is real, and propagating solutions result. For energies in the forbidden gap $E_c < E < E_v, k^2$ is negative, k is imaginary, and exponentially damped solutions result. It is these damped solutions with which we are concerned in tunneling problems. A typical experiment is to measure the tunneling current in a structure consisting of two metal layers separated by a thin insulating layer. The energy diagram for such a structure is shown in Fig. 2.

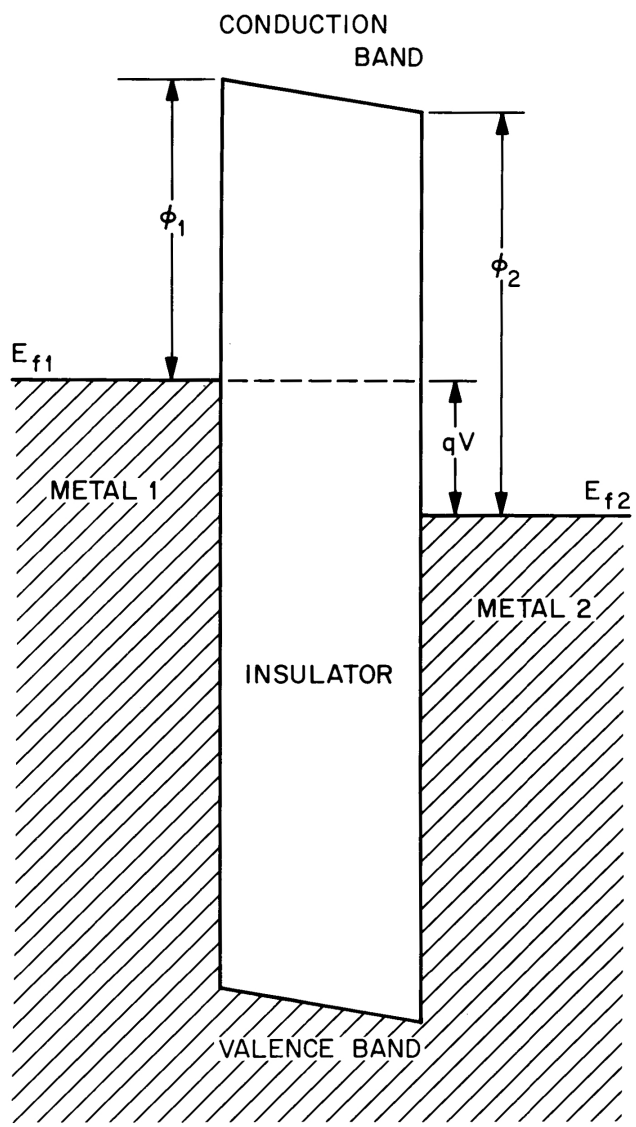

Figure 2: Energy diagram of metal-insulator-metal tunneling structure.

The tunneling current through such a structure at any particular applied voltage V is proportional to the tunneling probability P, which in turn is given by a WKB-type integral

$$P = \exp -2 \int_0^t k(x)\, dx, \tag{2}$$

where t is the insulator thickness and k is the imaginary part of the propagation vector. The dependence of k upon x arises from the dependence of k on E and the electric field in the insulator, which causes E to depend on x. For a uniform field E is proportional to x plus a constant, and the probability can be

rewritten

$$\log P = \frac{-2t}{\varphi_1 - \varphi_2 + qV} \int_{E_1}^{E_2} k(E)\, dE, \tag{3}$$

where E_1 and E_2 are, respectively, the initial and final state energies of the particular electron under consideration relative to the insulator conduction band.

Since normally we are considering energies in the upper half of the forbidden gap, k generally increases as E decreases. Since k appears in the exponent of the tunneling probability, electrons with higher energies contribute much more to the tunnel current than those with lower energies. However, above the Fermi level E_{f1}, we rapidly run out of electrons. Hence, for most experimental conditions the tunneling current is a very sharply peaked function at E_{f1}. Referring to Fig. 2 and defining our energy zero at the insulator conduction band edge E_c, we can write the tunneling probability

$$\log P = \frac{2t}{qV + \varphi_1 - \varphi_2} \int_{-\varphi_1}^{-\varphi_2 + qV} k(E)\, dE. \tag{4}$$

At this point, we can go no further without a knowledge of the dependence of k on E. It is clear from Fig. 1 that any analysis based upon the effective-mass approximation is doomed to dismal failure if the energies involved are an appreciable fraction of the forbidden gap, and even great quantities of mathematical manipulation do not serve to alleviate the problem. This point is the basis of a large portion of the disagreement between theory and experiment in the tunneling literature.

Two questions must be asked at this point:

1. Is there enough information in the experimental tunneling data to unambiguously determine the E versus k relation for the insulator being used?
2. Are enough self-consistency checks available to be sure that the E versus k curve so determined is real and not merely an agglomerated uncertainty factor?

The answer to both of these questions is, within broad limits, affirmative, and we will proceed on that basis.

From Eq. 4, we note that the logarithm of the tunneling probability is linear in the thickness t with a slope dependent upon the applied voltage through the limit on the integral. This dependence is shown schematically in Fig. 3.

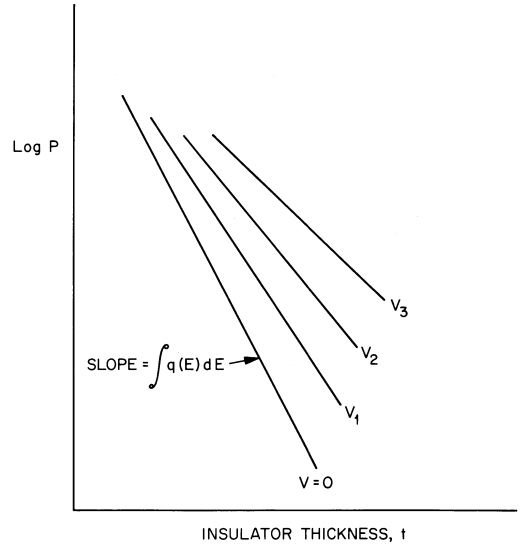

Figure 3: Dependence of tunneling probability on insulator thickness for different applied bias V.

From here the E versus k relationship can be determined directly. From Eq. 4, the slopes of the curves in Fig. 3 are given by

$$\text{slope} = \frac{\partial \log P}{\partial t} = \frac{2}{\varphi_1 - \varphi_2 + qV} \int_{-\varphi_1}^{\varphi_2 + qV} k(E)\, dE; \tag{5}$$

$k(E)$ itself may now be evaluated, as it is just the derivative of the integral with respect to its upper limit:

$$\frac{\Delta(\frac{1}{2}\,(\varphi_1 - \varphi_2 + qV) \times \text{slope})}{\Delta(qV)} = k(-\varphi_2 + qV). \tag{6}$$

Thus, the k versus E relationship is given directly by the differences in slope for curves of different voltages. The tunneling probability is subject to direct experimental measurement. At zero voltage, the small-signal tunnel resistance R of the sample and its capacitance C can be measured. It can be shown that [1]

$$P \propto 1/RC. \tag{7}$$

At applied biases larger than typically a few tenths of a volt, the tunneling probability is, to a good approximation, proportional to the current times the square of the insulator thickness [2]. Thus, curves similar to Fig. 3 are accessible by direct electrical measurement.

The relationship given by Eq. 5 and Eq. 7 is particularly direct and is demonstrated experimentally in Fig. 4. The data are from Al-AIN-Mg structures reported by Lewicki [3] and Lewicki and Mead [4]. The k versus E curve for these samples resulting from an analysis similar to that described above is shown in Fig 5. The k versus E curve is very much similar to what we sketched in Fig. 1, and its slope changes by more than a factor of two over the energy range involved in the tunneling. Thus, it is not surprising that calculations based upon an effective-mass approximation give thoroughly erroneous results.

We have now come to the point where we have (within the limits of the technique) a complete description of the system, and can check the self-consistency of the results.

1. The E versus k relation should be a property of the insulating material, and therefore not dependent on the electrode barrier energy φ. In Fig. 5, the results of the analysis are shown for two bias polarities where the φ's were different, and the same E versus k relation holds for both. Similar

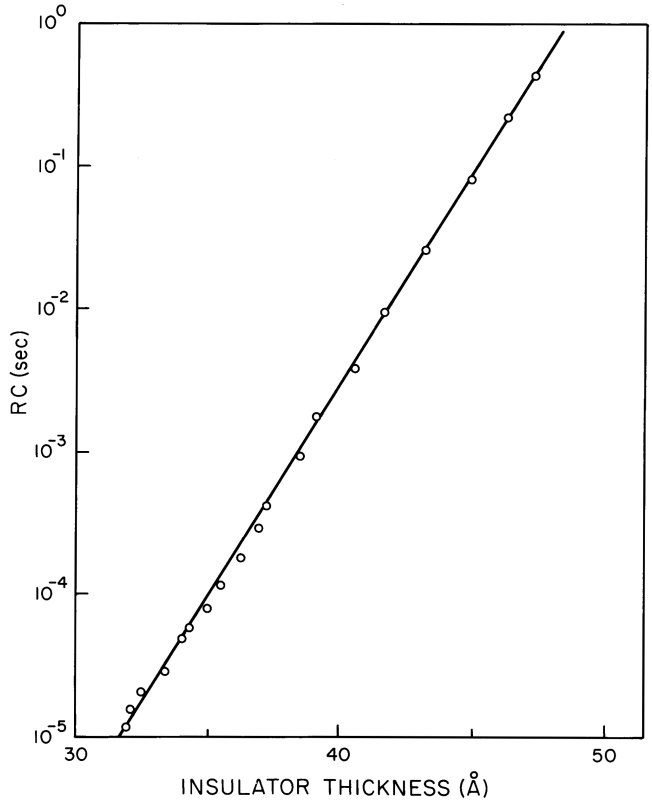

Figure 4: Product of low-frequency capacitance and zero bias tunneling resistance as a function of insulator thickness. This product is a direct measure of the tunneling probability.

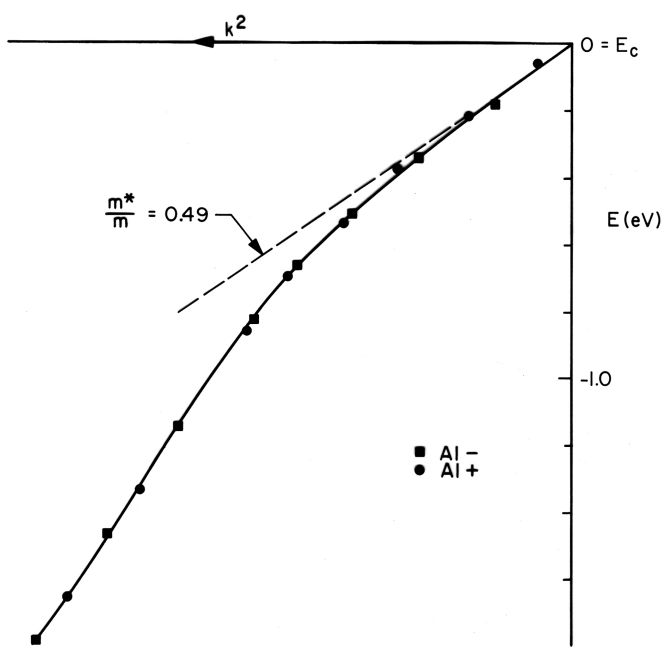

Figure 5: The $E - k$ relationship as derived by Lewicki on Al-AIN-Mg structures using the method outlined in the text. Note strong deviation from effective-mass approximation.

results obtained for other electrode materials where the barrier energies differ by even a larger amount. In the latter case, the volt-ampere curves are very different, and would not be expected to yield the same results unless the technique were self-consistent. This is an important point, and

should always be checked in each experimental situation.

2. The technique yields values for the barrier energies φ_1 and φ_2. These may be checked independently by two methods: (a) the cusps in the (small) temperature dependence of the tunnel current [5] and (b) threshold for internal photoemission. Both experiments have been done on the AIN samples, and the results agree with the $E - k$ method within experimental uncertainty.

3. Using the $E-k$ relation shown, it is possible to compute not only the form of the $I-V$ characteristics, but the absolute magnitude as well. When this is done, the $I - V$ curves *of both polarities* agree with those observed, and the magnitude is within a factor of two of that computed from the usual theoretical models.

Thus, we may conclude that within the limitation of the somewhat rough and ready method tunneling in thin films can be characterized in a simple and demonstrably self-consistent manner. Undoubtedly, details will accumulate and refinements of experiment and theory will ensue, but it is important to have the first-order ideas correct before such additions are attempted.

Exponentially attenuated wave functions are also important in other experimental situations. In particular, these states, like any other states, are either occupied or empty, and the charge stored in them can be appreciable. As an example, on the free surface of a semiconductor there can be one such state for every surface atom, or approximately 10^{14} per cm^2. If every one were occupied with one electronic charge, a field of 10^8 V/cm would result. Turning the argument around, a field of 10^6 V/cm terminating on the semiconductor surface would induce charge in only one percent of the available states. This serves to illustrate the powerful effect these states can have on the electronic nature of surfaces. A review of the interaction of these states at metal-semiconductor interfaces has been given previously, and will not be repeated here [6]. In addition, an excellent description of this effect on the semiconductor-vacuum surface is given by van Laar and Scheer [7].

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