¹⁵J. Kondo, in Solid State Physics, edited by H. Ehren-reich, F. Seitz, and D. Turnbull (Academic, New York, 1969), Vol. 23, p. 183; A. J. Heeger, *ibid.*, p. 284;
H. G. Howve and D. O. Van Ostenburg, Phys. Rev. Letters

26, 1020 (1971). ¹⁶Wolf and Losee (Ref. 9) introduced a Lorentzian smear-

ing of the Zeeman level. While the procedure has certain

PHYSICAL REVIEW B

validity for an energy range small compared with the Zeeman splitting (Δ) itself, they employed it over the entire integration range, where its validity was highly questionable.

¹⁷W. F. Brinkman, R. C. Dynes, and J. M. Rowell, J. Appl. Phys. <u>41</u>, 1915 (1970).

VOLUME 5, NUMBER 2

15 JANUARY 1972

Dielectric-Relaxation Currents in Insulators*

J. G. Simmons and G. W. Taylor

Electrical Engineering Department, University of Toronto, Toronto, Canada (Received 6 July 1971)

If at low temperatures a voltage bias is applied to an insulator containing traps, it is shown that the current flowing in the insulator is a non-steady-state dielectric-relaxation current (DRC) which is always greater than the steady-state current. If the sample is held at low temperatures, the DRC will prevail essentially indefinitely. However, if the temperature of the sample is raised, then over some narrow interval of temperature, centered around a temperature, say, T_m , the insulator and hence the current through the system relax quickly to the steady-state condition. Thus, at T_m , the DRC-vs-temperature characteristic exhibits a pronounced maximum. T_m is related to the depth of the trapping level below the bottom of the conduction band of the insulator, and the area under the DRC-vs-temperature characteristic is directly proportional to the trapping density.

In the study of the electrical properties of thinfilm insulators, one of the usual measurements is the activation energy of the conduction process. This is obtained by first cooling the sample to low temperatures and, with a constant-voltage bias on the electrodes, subsequently observing the current I as a function of increasing temperature T. A plot of $\ln I$ vs T^{-1} normally yields a straight line, the slope of which is a measure of the activation energy of the conduction process.¹ A second method, which yields detailed information about trapping levels in the insulator, is the thermally stimulated conductivity (TSC) technique.² In this case the insulator is cooled to low temperatures and the solid is stimulated by ultraviolet light, or other means, to excite (fill) some of the trapping levels above the equilibrium Fermi level E_F with electrons and those below E_F with holes. As the solid is heated, usually at a constant rate of temperature rise, pronounced peaks appear in the current (the voltage bias is held constant) at certain temperatures, which may be related to the energies of the excited trapping levels.²

Recently, several investigators³⁻⁶ have reported anomalous pronounced peaks in the current-vstemperature plots (see Fig. 1) when making conventional activation-energy measurements on thinfilm insulators. These peaks may be observed if the sample is cooled with its electrodes short circuited^{5,6} or open circuited.⁶ These peaks are essentially identical to those occurring in TSC measurements; yet the insulator is *not* optically stimulated prior to heating the insulator. It is the object of this paper to provide an explanation for this anomaly.

The basic principle underlying the explanation is that the current flowing in a highly resistive medium, particularly one containing traps, is, generally speaking, not a steady-state current *immediately* after the voltage is applied at low temperature. The current is, in fact, a dielectricrelaxation current (DRC), since the time taken for it to reach the steady-state value is determined by the dielectric-relaxation time of the system, which is a strong function of temperature. Furthermore, when traps are present in the medium, they essentially determine the dielectric-relaxation time of the system.

Consider the metal-insulator-metal system shown in Fig. 2(a). The insulator is assumed to be amorphous and thus would be expected to have acceptor- and donor-type traps distributed throughout its band gap.⁷ In order to simplify and expedite our arguments we assume that the distributed donor traps are lumped together to form a single trap level of density N_t , positioned at an energy E_t below the bottom of the conduction band. As far as the conduction process to be described is concerned, acceptor-type traps may be ignored. However, these types of traps are of significance when acting as compensation centers, since they have a role in determining the position of the equi-

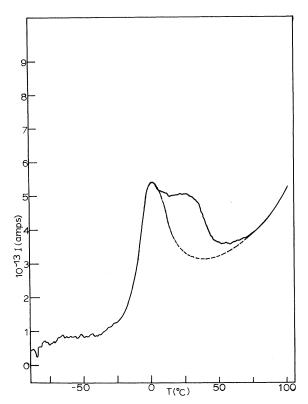


FIG. 1. DRC curve obtained from a silicon nitride film 800 Å thick. The sample was cooled to liquid-nitrogen temperature with the electrodes short circuited, and then heated at a rate of 0.2 degrees per second with 4 V applied. The dotted curve is the theoretical DRC curve [see (6)] for a *discrete* trapping level where $E_t = 0.75$ eV, $N_t = 10^{16}$ cm⁻³, and $\beta = 0.2$ degrees per second. Thus, from a comparison of the theoretical and experimental curves it will be apparent that the experimental peak is due to a distribution of trapping levels in the insulator, in which case the shape of the characteristic is a direct reflection of the trapping dis-tribution (Ref. 10). (The rising portion of the experimental curve at temperatures beyond the DRC curve is the steady-state current flowing in the sample.)

librium Fermi level. It is of little consequence here what degree of compensation is present, but we will assume for expediency that the density of compensating centers is $\frac{1}{2}N_t$. Hence the Fermi level is pinned at the donor-type center at all practical temperatures.^{8,9} (It is assumed that the free-carrier density is always much less than N_t .) Also, to expedite our explanation, we have assumed that the work functions of the insulator, ψ_i , and electrodes, ψ_m , are identical, so that when the electrodes are applied to the insulator the conduction bands are flat throughout the length of the insulator.¹⁰ Let us assume that the temperature is sufficiently high so that at all voltage biases the system reaches its steady-state condition [Fig. 2(c)] relatively quickly. Immediately after a voltage bias is applied to the system, the applied voltage is distributed linearly throughout the insulator, as shown in Fig. 2(b) and as evidenced by the straight Fermi level. The current flowing across the cathode is given by the modified Richardson-Schottky¹¹ expression

$$I = e \,\mu n \, F_c \, e^{\beta F_c^{1/2} / kT} \quad , \tag{1}$$

and the current in the insulator bulk outside the space-charge region is given by the Frenkel-Poole equation $^{12}\,$

$$I = e \,\mu n \, F_{\,b} \, e^{2\beta F_{\,b}^{\,1/\,2/\,kT}} \quad , \tag{2}$$

where

$$n = N_c e^{-E_t/kT} ,$$

$$\beta = e \left(e/\pi \epsilon_0 K \right)^{1/2}$$

 N_c is the effective density of states in the conduction band, μ is the electronic mobility, F_c and F_b are the electric fields at the interface and in the bulk respectively, and K is the high-frequency dielectric constant of the insulator. Thus, since initially $F_c = F_b$, the electronic current flowing into the cathode is less than that flowing out at the anode; hence a positive space-charge region is created in the insulator adjacent to the cathode. As this spacecharge region grows, the field at the cathode, F_c , increases and the field outside the space-charge region, F_b , decreases, as shown in Fig. 2(c). This relaxation process continues until the cur-

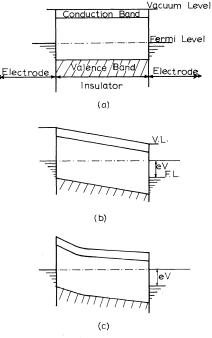


FIG. 2. Energy diagram of idealized amorphous insulator (a) under zero bias, (b) immediately after a voltage V is applied, and (c) with voltage bias applied and the system in the steady-state condition.

rent is constant throughout the system. When this condition exists, the field at the cathode-insulator interface is approximately *twice* that in the neutral region of the insulator, as will be apparent from an inspection of (1) and (2). Also, the steady-state width of the space-charge region adjacent to the cathode is greater the greater the voltage bias. However, this process cannot continue indefinitely, since at sufficiently high voltage bias the barrier at the cathode-insulator interface will become permeable to tunneling electrons. The tunnel current increases much faster with increasing field than does the Frenkel-Poole effect, with the result that an electrode-limited-to-bulklimited transition occurs in the conduction process.¹³ At the onset of this process, the spacecharge region becomes only very weakly dependent on the applied voltage.

Next, consider what happens if the sample is cooled to a low temperature T_0 without a voltage bias on the electrodes and then, at the low temperature, a fixed voltage bias is applied to the electrodes. Normally at low temperature the emission of charge from the traps will be negligible; thus it will take the system an extremely long time to relax to the steady state. The time t_r for the insulator to relax to the steady state is given approximately by

$$t_{\mu} = \nu^{-1} e^{E_t / kT}$$
 (3)

where ν is the attempt-to-escape frequency, k is Boltzmann's constant, and T is the temperature (°K). Assuming T = 100 °K, $E_t = \frac{1}{2}$ eV, and $\nu = 10^{11}$ sec, then $t_r \simeq 10^{16}$ sec. Thus it takes the system an inordinately long time to relax at low temperatures. This means that when a voltage is applied to the system it is dropped uniformly throughout the solid [see Fig. 2(b)] and normally remains so during the course of the time it takes to make an I-V measurement. Now, if instead of holding the sample at a constant low temperature it is heated with a fixed voltage applied and at a constant rate, B degrees per second, that is,

$$T = Bt + T_0 , \qquad (4)$$

the trap level will become an effective emitter of electrons at a temperature T_m given by⁶

$$BE_{t}/kT_{m}^{2} = \nu e^{-E_{t}/kT_{m}}$$
 (5)

As a result, around this temperature the dielectric begins to relax quickly from the non-steady-state [depicted in Fig. 2(b)] to the steady state [shown

*Work supported by Defence Research Board of Canada, Grant No. 9512-33, and National Research Council of Canada. in Fig. 2(c)], during which process the charge within the insulator is redistributed as required by steady-state conditions. The charge released in forming the space-charge region is typically 10^{10} -10¹³ electrons per square centimeter of device area, the great majority of which escapes from the system in a matter of seconds. Hence the current flowing in the external circuit associated with charge redistribution is much larger than, and superposed on, the current supplied from the cathode, and it ceases when the charge redistribution within the insulator ceases. Thus the DRC-vs-temperature characteristic exhibits a maximum. The maximum occurs at a temperature T_m given by (5). In this case, however, it is noted that, contrary to conventional thermally stimulated currents, the sample is not stimulated at the start of the heating process. It can be shown⁶ that if the insulator contains only a single *discrete* trap, the current at constant voltage is given by (see Fig. 1)

$$I(T) = \frac{e\lambda}{4} \frac{N_t}{t_r} \exp\left(-\frac{kT^2}{B(E_t + kT)t_r}\right) \quad , \tag{6}$$

where λ is the space-charge-region width. Furthermore, the area A under the curve is related to the charge Q released from the insulator (charge contained in the space-charge region) as follows:

$$\int_{T_1}^{T_2} I dT = B \int_{t_1}^{t_2} I dt = B Q = A , \qquad (7)$$

where T_1 and T_2 are the temperatures corresponding to the beginning and end of the process¹⁴ and t_1 and t_2 are the times corresponding to T_1 and T_2 .

It will be noted that if a voltage bias is applied before the sample is cooled to low temperature and then the sample temperature raised with the same voltage bias applied, there will be no observable DRC maximum, since the sample will be essentially in its steady-state condition at all times during the experiment¹⁵ [see Fig. 2(c)]. It will also be apparent that the greater the applied voltage bias, the greater is the area under DRC curve; also the area under the curve is proportional to *B*. Finally, the depth of the trap below the bottom of the conduction band, as determined from (5), must be independent of *B* and the applied voltage if our premise is correct. All of these points have indeed been experimentally confirmed.

A complete treatment of dielectric-relaxation effects and associated phenomena in insulators containing distributed traps and blocking contacts will be given elsewhere.

¹J. G. Schnug, A. C. Lilley, and B. Lowitz, Phys. Rev. B 1, 4811 (1970).

²G. A. Dussel and R. H. Bube, Phys. Rev. <u>155</u>, 764 (1967).

³E. J. M. Kendall, Can. J. Phys. <u>46</u>, 2509 (1968).

⁴J. R. Yeargan and H. L. Taylor, J. Electrochem. Soc. <u>115</u>, 273 (1968).

⁵R. B. Cavanagh (private communication).

 6 J. G. Simmons and G. Taylor, Phys. Rev. B (to be published).

⁷M. L. Cohen, H. Fritzsche, and S. R. Ovshinsky, Phys. Rev. Letters <u>22</u>, 1065 (1969).

⁸J. G. Simmons, J. Phys. Chem. Solids <u>32</u>, 2581 (1971). ⁹The fact that the Fermi level is essentially temperature independent likens our insulator model to that of a real amorphous solid in which the Fermi level is also only very slightly temperature dependent (see Ref. 8 for further details).

¹⁰Effect of blocking contacts at the metal-insulator interface are to be treated elsewhere: J. G. Simmons and G. W. Taylor (unpublished).

¹¹J. G. Simmons, Phys. Rev. Letters <u>15</u>, 967 (1965).

¹²J. Frenkel, Phys. Rev. <u>54</u>, 647 (1938).

¹³J. G. Simmons, Phys. Rev. <u>166</u>, 912 (1968).

¹⁴The DRC flows in the system even in the temperature range $T_0 \ge T \ge T_1$ but is very small and is apparent only on a $\ln I$ -vs-T plot. On a linear I-vs-T plot the DRC is apparent only for temperatures close to T_e .

¹⁵This fact, together with the observation that the DRC curve is observed when the sample is cooled under shortor open-circuit conditions, eliminates the possibility that the effect is due to the filling of the traps by electrons injected from the electrodes.

PHYSICAL REVIEW B

VOLUME 5, NUMBER 2

15 JANUARY 1972

Exact Solution of the One-Dimensional Schrödinger Equation with δ -Function Potentials of Arbitrary Position and Strength*

John F. Reading[†]

Department of Physics, Texas A & M University, College Station, Texas 77843

and

James L. Sigel Department of Physics, Northeastern University, Boston, Massachusetts 02115 (Received 25 August 1971)

The exact solution to the one-dimensional Schrödinger equation which describes the motion of a particle scattering off a finite set of δ -function potentials of *arbitrary strengths* and *positions* is found. The behavior of the *T* matrix both on and off the energy shell is also precisely given. Localization of states is discussed.

I. INTRODUCTION

Recently a great deal of work¹ has been done on the problem of understanding the electronic states of a system in which the atomic scattering sites are randomly located. The importance of these studies in the field of semiconductor physics is well known. The mathematical difficulties involved in this problem have made it necessary to look into its one-dimensional version²⁻⁴ in hopes of getting some insight into the important features, so that extraneous complexities can be avoided in the threedimensional case.

Even with its simplifications the one-dimensional case has not proven to be trivial in nature and the work in this area has needed to be put on a firmer basis. In this paper we hope we have done this by providing an *exact* solution to the Schrödinger equation for an electron moving in one dimension in the presence of a set of δ -function potentials of arbitrary strengths and positions. The solution which we present has the feature that a clear delineation is made between terms that are made small due to incoherence effects, in the case of a random distribution of scattering sites, and those that are not. This feature of our solution makes it useful for an understanding of how wave functions grow inside the chain of scattering sites and thus it is applicable to the study of the all-important problem of localization.

In Sec. II we present our solution to the integral form of the Schrödinger equation. In Sec. III we recognize the fact that to obtain the wave function we did not have to completely invert the matrix M[defined by (2.5)]; we complete this task and show that the Fredholm determinant, i.e., det M, has, for positive energy, a magnitude greater than unity. With this inverse of M, we obtain, as well, the Tmatrix both on and off the energy shell and briefly discuss its connection with the evaluation of transport properties and the density of states in a specimen. Section IV is devoted to a discussion of some aspects of the problem of localization. We point out in that section that for positive energies, where $|\det M| \ge 1$, there can, for a finite chain of scattering sites, be no states which vanish at $\pm \infty$; thus no precisely localized states exist. For a finite chain, localization at positive energies is always, formally, only approximate.

In Appendix A, we discuss other forms of the solution found in Sec. II, while in Appendix B, we make the connection between our results and the