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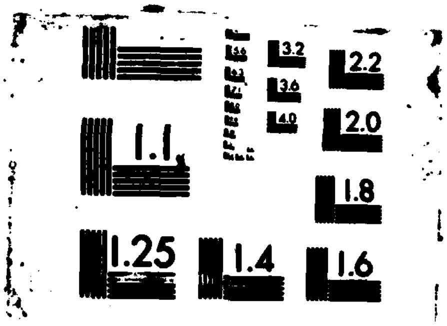

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The problem of recombination in insulators, especially thermally grown SiO_2, is an important part of the radiation response of microelectronic circuits. This report treats the geminate recombination process between an isolated electron-ion pair in the presence of an applied field. Specifically, the Onsager solution of the Smoluchowski equation has been programmed for numerical computation. The program has been applied to thermally grown SiO_2, and the results are presented as a function of applied field for several temperatures. A mean initial separation between negative and positive charges must be assumed, and the sensitivity of the result to this assumption is examined.

The model results predict very little temperature dependence except at very low fields. These results will be compared with measurements in the future. Keywords; Metal Oxide Semiconductors;

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FOREWORD

The manuscript of this report was completed by Dr. George A. Ausman, Jr., in late 1975. However, it was never published, mostly because of the untimely death of the author. We, his coworkers, have used the results presented here from time to time. Although other investigators have since gone beyond these results in some ways, we believe that this work remains a unique contribution which should be generally available.

At this time we are preparing a chapter for a book scheduled for publication in 1987 (tentatively titled Radiation Effects in MOS Devices and Circuits, edited by T. P. Ma and P. V. Dressendorfer, published by John Wiley & Sons). This chapter will deal with the geminate recombination model, among other subjects. We believe the work of Dr. Ausman deserves a place in this discussion. For this reason, we are publishing it now.

Timothy R. Oldham
F. Barry McLean
H. Edwin Boesch, Jr.

CONTENTS

FIGURES

1. INTRODUCTION

Radiation, such as that produced by high-energy electrons or photons, excites electron-hole pairs in a dielectric medium. The excited electrons rapidly come to thermal equilibrium in the lattice. Typical thermalization distances between an electron and its original ion or hole are of the order of 50 to 100 Å.* Following excitation and subsequent thermalization of the electrons, many of the initially created electron-hole pairs undergo recombination on a time scale of picoseconds.[1] The fraction of electrons escaping initial recombination is an increasing function of the applied electric field and also depends on the initial separation distance, temperature, and density of excited pairs. There are two basic mechanisms of initial recombination: columnar and geminate. If there is strong overlap between the spheres of influence of adjacent electron-hole pairs along the path of the ionizing particle, then homogeneous bimolecular recombination occurs within a column whose axis is the path of the primary ionizing particle. This type of recombination is called columnar recombination, the theory of which was developed by Jaffe.[2] If there is very little overlap between the spheres of influence of adjacent electron-hole pairs, then the individual electron-hole pairs are essentially isolated and geminate recombination occurs (recombination of an electron with its parent ion). The theory of geminate recombination was developed by Onsager.[3] Since the total net motion of the positive and negative charges during the initial recombination process is zero, the net current or charge transfer is zero. Those charges that escape initial recombination are able to contribute to observable charge transport processes.

The application of the columnar model of recombination to current versus field data in SiO_2 was discussed in a previous paper.[4] The Smoluchowski equation, which describes the time-dependent neutralization of an isolated electron-ion pair (geminate recombination) in a dielectric medium, was solved in a previous report[1] for the case of zero applied electric field. Onsager[3] was the first to obtain the steady-state solution (i.e., $t \rightarrow \infty$) to the Smoluchowski equation. He derived the important result that, in the absence of an applied electric field, the probability that the electron-ion pair will ultimately escape mutual neutralization is given by $\exp(-r_c/r)$, where r_c is the so-called Onsager "critical radius" for recombination and r is the initial separation of the electron and positive ion. Onsager also obtained the steady state solution in the presence of an applied electric field. This latter solution will be explored in detail in this report.

---

[1] G. A. Ausman, Jr., Annual Report of Conference on Electrical Insulation and Dielectric Phenomena (1973), p 456; and Harry Diamond Laboratories HDL-TR-1662 (April 1974).

[2] G. Jaffe, Ann. Phys. (Leipz.) 42 (1913), p 303.

[3] L. Onsager, Phys. Rev. 54 (1938), p 554.

[4] G. A. Ausman, Jr., and F. B. McLean, Appl. Phys. Lett. 26 (1975), p 173.

*1 Å = 0.1 nm.

2. ANALYSIS

For the geminate recombination process to be valid it is assumed that, following irradiation and subsequent thermalization of the electrons, the dielectric medium can be treated as consisting of isolated electron-ion pairs. Under this assumption, one can describe the recombination at early times by considering a single isolated electron-ion pair. The motion of the two charges of opposite signs is governed by the competing processes of mutual Coulomb attraction, the random walk in a dielectric medium, and drift in an applied electric field. The first process tends to bring the two charges together, whereas the latter two tend to separate them. The random walk is approximated by a diffusion term in the Smoluchowski equation. (A more detailed discussion of the Smoluchowski equation appears elsewhere.[1]) Onsager[3] has shown that the probability for ultimate escape ($t \to \infty$) of the electron-ion pair is given by

$$P(r,E,\theta) = \exp[-\beta r(1 + \cos\theta)] \times$$

$$\int_{r_c/r}^{\infty} ds \, \exp(-s) J_0 \{ 2[-\beta r(1 + \cos\theta)s]^{1/2} \} \quad . \tag{1}$$

In the above equation, r is the initial separation distance of the electron-ion pair, E is the electric field, θ is the angle between the electric field and the line joining the electron-ion pair, $\beta = (e/2kT)E$, $r_c = e^2/\epsilon kT$, e is the electronic charge, k is Boltzmann's constant, and T is the temperature. J_0 is the ordinary Bessel function of order zero and is related to the modified Bessel function of order zero, I_0, by

$$J_0(iz) = I_0(z) \quad . \tag{2}$$

In comparing the predictions with experiment, we assume that the initial thermalization of the electrons produces a practically isotropic distribution of directions about the parent ions. Therefore the quantity of practical interest is

$$P(r,E) = \langle P(r,E,\theta) \rangle = \frac{1}{\pi} \int_0^{\pi} d\theta \, P(r,E,\theta)$$

$$= \frac{1}{\pi} \int_0^{\pi} d\theta \, \exp[-\beta r(1 + \cos\theta)] \times$$

$$\int_{r_c/r}^{\infty} ds \, \exp(-s) I_0 \{ 2[\beta r(1 + \cos\theta)s]^{1/2} \} \quad . \tag{3}$$

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[1] G. A. Ausman, Jr., Annual Report of Conference on Electrical Insulation and Dielectric Phenomena (1973), p 456; and Harry Diamond Laboratories HDL-TR-1662 (April 1974).

[3] L. Onsager, Phys. Rev. 54 (1938), p 554.

An expansion of equation (3) in a power series of the electric field yields, to first order,

$$P(r,E) = \exp(-r_c/r) <1 + \beta r_c(1 + \cos\theta)>$$

$$= \exp(-r_c/r)(1 + \beta r_c) \,. \quad (4)$$

An important consequence of this result is that for sufficiently low fields, such that equation (4) is a valid approximation, the relative effect of the field is independent of the initial separation distance r. In fact, a plot of equation (4) yields a slope/intercept ratio,

$$\text{slope/intercept} = 1 + \beta r_c = 1 + (e^3/2\varepsilon k^2T^2)E \,. \quad (5)$$

Equation (5) depends only on the material parameters ε and T. This very useful relationship has been used by many investigators to test the applicability of the geminate recombination model to given experimental conditions. In practice, the yield of charge is measured as a function of applied electric field for fields sufficiently low that a linear relationship is obtained. The experimentally obtained slope/intercept ratio is then compared with that predicted by equation (5). In the calculations presented below, which take into account the complete field dependence of the geminate escape probability, it is shown that the slope/intercept test can sometimes be quite misleading in interpreting experimental data.

Equation (3) was programmed for numerical computation. For large x, $I_0(x) \sim e^x$. Since for large electric fields (large β) all exponential factors have large arguments, overflow (or underflow) occurs for sufficiently large β unless all exponential factors are combined into a single exponential factor before any integration is performed. To accomplish this it was necessary to place the exponential involving only the variable θ inside the integral over s. The double integration was then performed numerically with the use of Simpson's rule. The basic input parameters to the program are the dielectric constant of the material, the initial separation distance, and the temperature. The program computes the escape probability as a function of electric field over a range specified by the user.

3. RESULTS AND DISCUSSION

The escape probability as a function of electric field, calculated from equation (3), is shown in figures 1 through 5 for various values of the initial separation distance, r, and temperature, T. Figures 1 through 3 give the field dependence of the escape probability for the three values of r = 50, 80, and 100 Å, and for the temperatures 80, 193, and 293 K. Figure 4 displays the explicit dependence on separation distance at 293 K.

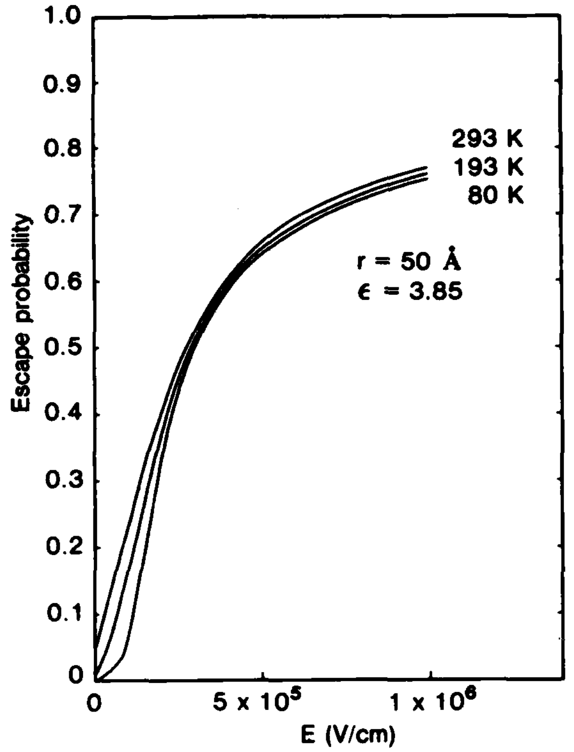

Figure 1. Escape probability as a function of field for initial electron-hole separation of 5 nm at different temperatures.

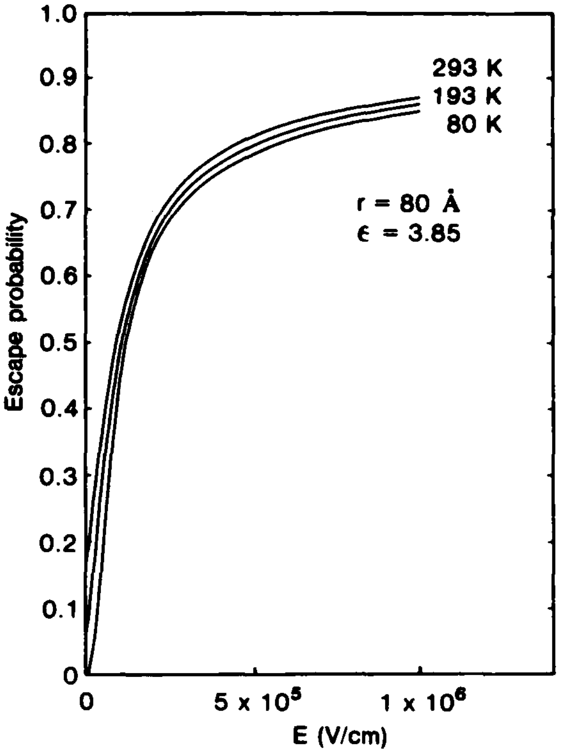

Figure 2. Escape probability as a function of field for initial electron-hole separation of 8 nm at different temperatures.

The danger, referred to earlier, of applying the slope/intercept test to experimental data is illustrated in figure 5. In this figure an expanded field scale is used. The dashed lines are an extrapolation of the linear regime. Since in many experiments it is very difficult to obtain data in the true, low-field linear regime, it is possible to misinterpret the data by assuming that the data in the field regime just above 5×10^4 V/cm (frequently an experimental lower limit) are in the linear regime. The application of the slope/intercept test to the 80 K data in this field regime actually leads to a *negative* slope/intercept ratio. Even at 193 and 293 K, a slight amount of scatter in the experimental data could lead one to misinterpret the location of the linear regime and, in turn, to obtain erroneous values for the slope/intercept ratio. Figure 1, the 50-A case, illustrates this danger of misinterpretation even more dramatically.

4. CONCLUSION

Since the preceding discussion illustrates the difficulties in applying the slope/intercept test to experimental data, apparently the only conclusive procedure for determining the applicability of the geminate recombination model to a particular experimental situation is to attempt to fit the data over the entire field range by equation (3). The only variable parameter in this model is the initial electron-ion separation distance.

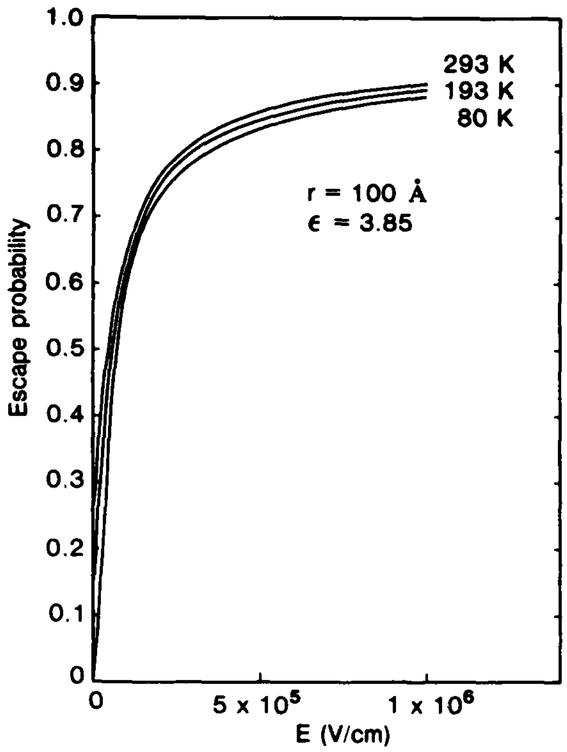

Figure 3. Escape probability as a function of field for initial electron-hole separation of 10 nm at different temperatures.

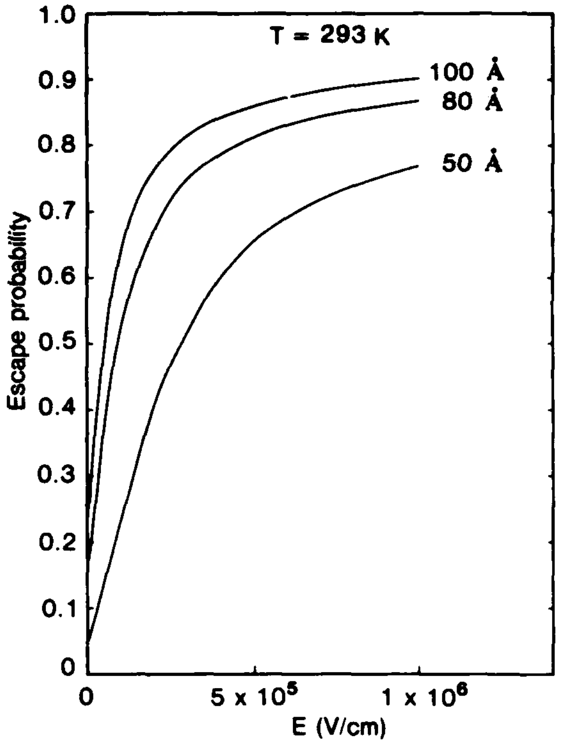

Figure 4. Escape probability as a function of field at room temperature for different initial electron-hole separations.

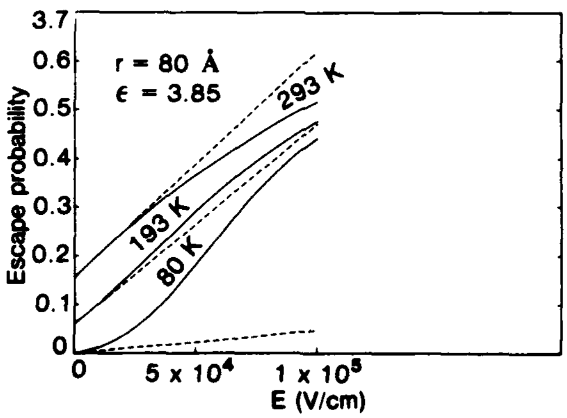

Figure 5. Escape probability plotted on an expanded field scale. Dashed lines are extrapolations of the low-field linear slope region.

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