AD-A194 258 A STUDY OF ELECTRONIC TRANSPORT AND BREAKDOWN IN SIO2 1/1
(U) ARIZONA STATE UNIV TEMPE CENTER FOR SOLID STATE
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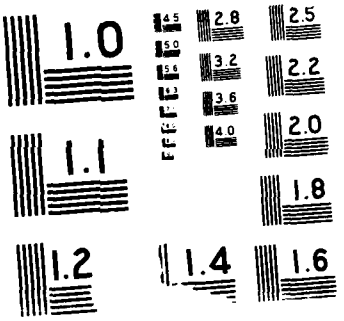
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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER N88.F1	2. GOVT ACCESSION NO. N/A	3. RECIPIENT'S CATALOG NUMBER N/A
4. TITLE (and Subtitle) A study of Electronic Transport and Breakdown in SiO_2		5. TYPE OF REPORT & PERIOD COVERED Final
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) D.K. Ferry		8. CONTRACT OR GRANT NUMBER(s) N00014-86-K-0541
9. PERFORMING ORGANIZATION NAME AND ADDRESS Center for Solid State Electronics Research Arizona State University Tempe, AZ 85287		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research (414) 800 North Quincy Arlington, VA 22217		12. REPORT DATE 1 March 1988
		13. NUMBER OF PAGES 9
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

RIBUTION STATEMENT (of this Report)

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RIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

LEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Tunneling, breakdown, transport

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Transport of electrons in silicon dioxide, at high electric fields, has been of much interest for quite some time. In spite of this, the role of various scattering processes has not yet been sorted out. At low fields, electrons show a mobility in the 20-30 cm^2/V-sec range, and at high fields (of the order of 1 MV/cm) begin to exhibit hot carrier effects. The polar modes are the dominant electron scatterers for fields up to 1.5-2 MV/cm, and beyond this, runaway begins to occur. Experimentally, it is found that the electron distribution function stabilizes at an average energy around 3 eV for fields above 3 MV/cm, which requires the onset of additional scattering processes.

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HIGH FIELD TRANSPORT IN SiO_2

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INTRODUCTION

For a great many years, the transport of electrons in amorphous silicon dioxide has been of interest to the electronics community. This interest stems from the importance of this material as an insulator for microelectronics. Primarily, silicon dioxide has been studied for its structure and conductivity, as well as breakdown strength, due to the high voltages applied across the thin layers found in gate oxides of MOS devices. For VLSI, and the new ULSI, fields in the insulator are expected to be on the order of a few MV/cm, and thus relatively close to electrical breakdown.

From the early studies of the transport through silicon dioxide, it was thought that the scattering of electrons was dominated by the polar optical phonon interaction (Lynch 1972, Thornber and Feynman 1970, Ferry 1979). Through the emission of optical phonons, electrons can lose the energy which they gain in the electric field, and it was felt that this interaction was sufficiently strong to prevent the electrons from suffering polar runaway. This would imply that the electron distribution was stabilized at an average energy below the optical phonon energy (0.15 eV). It is now known that this is not the case. From both experimental (Theis et al. 1983, 1984) and theoretical studies (Fitting and Friemann 1982), it is now known that the polar phonons are unable to stabilize the distribution above 1.5-2.0 MV/cm. This field is well below that at which silicon dioxide is found to break down; so that we are left with the question as to what then determines the stabilization of the electron distribution function to avoid breakdown?

Fischetti (1984) suggested that umklapp processes involving the acoustic phonons provided an additional scattering mechanism, and that this mechanism was sufficiently strong to stabilize the distribution, with an average energy in the 2-5 eV range found experimentally. Porod and Ferry (1985a), on the other hand, introduced scattering to satellite valleys of the conduction band, which in turn stabilized the distribution and could also fit the experimental data. The key factor in each of these approaches, studied by ensemble Monte Carlo calculations, was the introduction of an additional large density of states, which causes the large scattering rates necessary to stabilize the distribution.

In this paper, the current understanding of the transport and scattering processes will be reviewed. In particular, the role of umklapp processes and intervalley processes will be discussed in the next two sections, which deal with the general problems of the electron-phonon interaction. Impact ionization is treated in the following section. Finally, a short discussion of the modifications expected with quantization will be presented.

THE ELECTRON-PHONON INTERACTION

The general features of the electronic structure for various crystalline modifications of silicon dioxide are actually quite similar despite their different crystal structures. This tends to point out the absolute importance of the short range order in determining the essential features of the electronic structure. We can actually carry this forward to the amorphous phase as well. In fact, one of the interesting apects of silicon dioxide is that the mobility of the electrons is quite large when compared to the expected values for insulators, and is actually much closer to that expected for a low mobility, wide band-gap semiconductor. Indeed, it now appears that the mean-free path for the electrons is of the order, or smaller than the grain size, or ordering length of the material. As a consequence we really expect the details of the electron-phonon interaction to be described by the general lattice theory of crystalline solids (but modified in detail appropriate to the lack of long-range order in the amorphous phase).

Earlier attempts to treat the scattering by LO phonons in silicon dioxide led to relatively good agreement between low field mobilities found experimentally and theoretically. The major scattering processes, at least at low electric field, were previously shown to be the LO modes of the lattice (Lynch, 1972). There are two principle modes that interact, at energies of 0.06 and 0.153 eV, and these split the total polar coupling given by the difference between the optical and static dielectric constants. However, there are many other scattering mechanisms that could play a role, especially at high electric fields. To this end, it is probably well worth while to review briefly the electron-phonon interaction generally.

The relatively high mobility of most semiconductors, and even to a major extent in a material such as silicon dioxide, indicates that the electron-phonon interaction can be treated in perturbation theory. The basis of this simplification is the adiabatic approximation in which the motion of the electrons and the lattice are separated. The interaction term may then be expanded into the various interaction terms (Vogl, 1976). In a primitive sense, we can write the interaction orders as

$$M = A/q + Bq^0 + Cq + \ldots , \qquad (1)$$

i.e. as a series in q. In purely homopolar materials, such as Si and Ge, the leading term has A=0, since this term depends upon the dipole fields existing within the unit cell. Thus, only those crystals lacking an inversion center have this term present. Silicon dioxide certainly fits tnis mold. This first term gives rise to the longitudinal polar optical phonon scattering for the optical modes and to piezoelectric scattering for the acoustic modes. The former is the dominant scattering process usually in materials in which it can occur, at least over a portion of the energy range spanned by the electrons. The latter is usually only found at lower temperatures, but can be significant as a scattering mechanism.

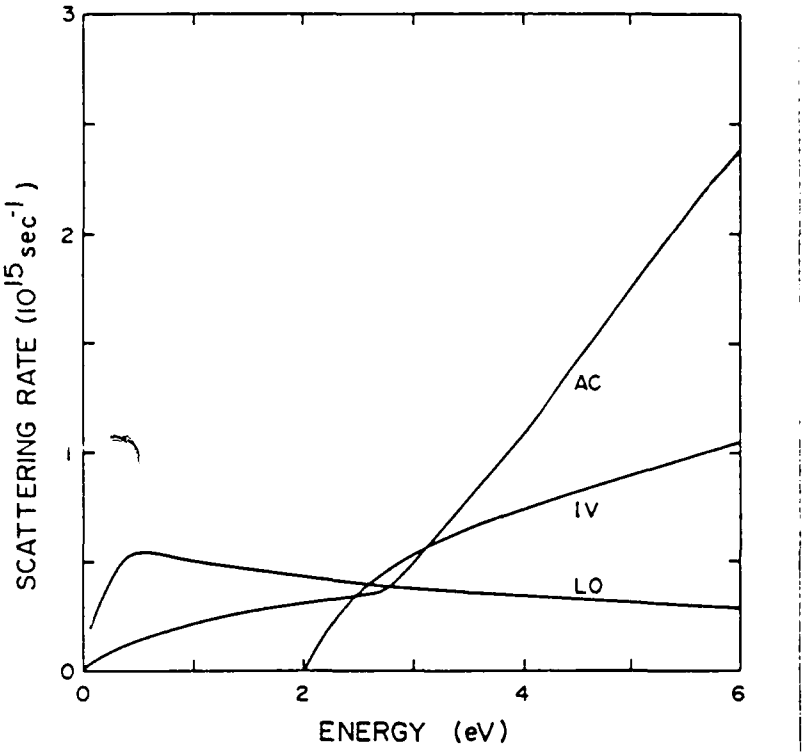

Fig. 1. Scattering rates used in the present study.

The zero-order term always vanishes for the acoustic modes, as this amounts to a uniform displacement of the entire crystal. In the optical modes, however, it leads to non-polar optical phonon scattering, where the phonons arise near the zone center. It is also responsible for intervalley scattering, in which the phonon is a large momentum phonon, and is usually an umklapp process. In many cases, these interactions and the appropriate phonon branches must be carefully screened for the appropriate symmetry.

The first-order term gives rise to the deformation potential interaction for the acoustic modes. Of interest here is also the fact that umklapp processes have been used to treat the acoustic interaction at high energies as well (Fischetti, 1984). This term, and the optical branch interaction as well, has also been shown to be important for intervalley processes in which the zero-order interaction is symmetry forbidden (Ferry, 1976), such as in Si itself. The higher order terms give rise to multi-pole scattering terms, but are not thought to contribute significantly to scattering in semiconductors.

The form of the matrix elements, and consequently the scattering rates, has been worked out for most of the lower order scattering processes for quite some time. They can be found e.g. in Conwell (1967) and Ridley (1982). What are not so well known are the values for the various "coupling constants" required to give numerical values to the scattering rates. In Fig. 1, the scattering rates for silicon dioxide are plotted. All of the various emission and absorption processes for the two dominant polar modes are gathered together for the curve marked LO. The coupling constant for each mode is determined by the known split of the dielectric function between the two dominant modes and is not further adjusted. The acoustic curve (AC) includes piezoelectric, deformation potential and the umklapp process. Piezoelectric scattering is relatively

weak, being only about 10% of the acoustic mode at low energies. The acoustic deformation potential here is 10 eV. Throughout the present work, the electron mass is taken to be 0.7m at low energies and 1.0m at high energies, in keeping with the recent estimates of Fischetti et al. (1987). The strength of the umklapp process was adjusted to a value in keeping with the scattering strength used by the latter authors, but the form of the interaction differs somewhat to account for the actual threshold in this process. In addition, scattering by the nonpolar optical phonon to a second set of valleys has been included (IV). The details of this interaction are in keeping with the earlier reports of its use (Porod and Ferry, 1985a). These scattering rates give good agreement with the low field mobility reported by Hughes (1978). Yet, it is important to note that almost none of the parameters, which describe the coupling between the electrons and the lattice have actually been experimentally determined.

HIGH FIELD STABILITY

The transport through silicon dioxide has been studied by the use of an ensemble Monte Carlo technique in which the scattering mechanisms of Fig. 1 are incorporated. Typically, the ensemble contains about 2000 electrons, which is a large enough number to give meaningful ensemble averages for the kinetic coefficients, such as average energy. The electrons are treated as if the structure is a free electron band structure, with the sole exception of the varying effective mass, as discussed above. Still, this band structure introduces considerable multiplicity in the bands at higher energy, due to the pseudo-periodicity of the crystalline structure.

The significant factor in Fig. 1 is the presence of the two scattering mechanisms which lead to very high scattering rates at high electron energies. In the absence of these scattering processes, the electron distribution function becomes unstable above 1.5-2.0 MV/cm. By unstable, we mean that the average energy of the carrier ensemble increases very rapidly. It is the presence of the additional (and large) scattering processes which are responsible for stabilizing the distribution. We can see this in Fig. 2, which displays the average energy found for the electrons as a function of the electric field. The gray area is the range of average energies determined experimentally by Theis et al. (1983,1984), Fischetti et al. (1985), and DiMaria et al. (1986). The curve marked 1 neglects the intervalley processes. We note that the scattering rate for the umklapp processes (Fig. 1) is actually slightly weaker than that used by Fischetti (1984), and the curve tends to begin to become unstable above about 8 MV/cm. While this curve lies at the bottom of the range found experimentally (up to 8 MV/cm), weakening the umklapp process would cause the entire distribution to become unstable. The curves marked 2 and 2′ neglect the umklapp process, but do include the intervalley process at various strengths. Curve 2 increases the scattering by 50% to overcome for the loss of the umklapp process, but clearly stabilizes the energy at a value well below that found experimentally. On the other hand, curve 2′ weakens the intervalley process over that shown in Fig. 1 by this same factor. In the latter case, the distribution becomes unstable already at 3-4 MV/cm. Curve 3 includes all of the various scattering processes, with the strengths shown in Fig. 1. This curve lies somewhat below the experimental data at intermediate fields. Judicious adjustment of the various parameters, such as increasing the onset of intervalley scattering from 2 to 3 eV, allows us to actually put the entire curve within the experimental area.

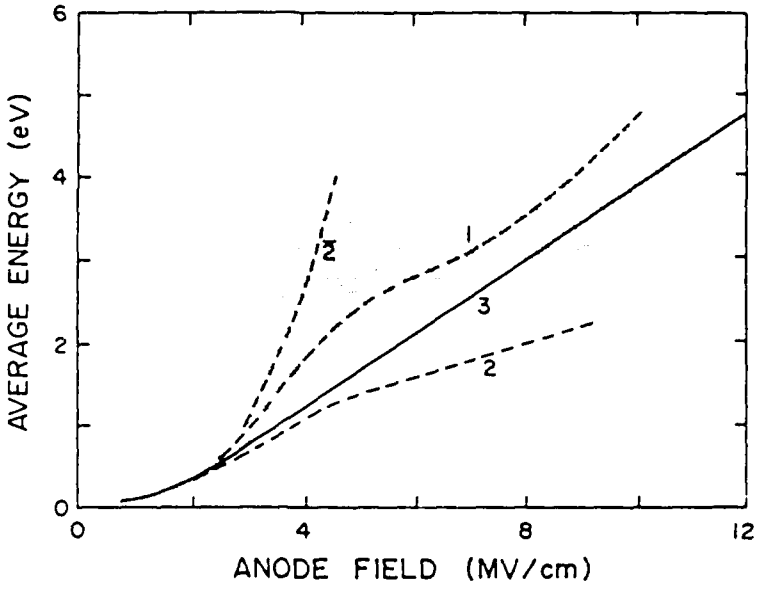

Fig. 2. The average energy calculated from the ensemble Monte Carlo model. The shaded area is the range of experimental curves, while the various curves are discussed in the text.

By judicious adjustment of the coupling constants and the threshold energies for the high energy scattering processes, one can obtain relatively good agreement with the range of experimental data on the average energy of the electron distribution. However, what does this mean in light of the fact, mentioned above, that we really don't know the proper values for most of the coupling constants used in the theory. Indeed, the message from Fig. 2 is that it is primarily the extra density of states incorporated in the high energy scatterers, and not the details of the physics of these scatterers, that leads to the resulting stability of the electron distribution. What has been achieved is the essential proof that an additional scattering process, of relatively high scattering rate, can work to stabilize the distribution of carriers. Moreover, the average energy of the resulting distribution is not correlated to any particular parameter of the scattering process, in contrast to the result expected for polar scattering. On the other hand, this does not deter us from drawing some very important conclusions about breakdown from this model, which will be discussed below.

QUANTUM EFFECTS

One needs, in principle, to consider the fact that the scattering indicated in Fig. 1 is certainly not weak scattering, particularly at high electric fields, and high electron energies. The presence of such strong scattering means that we must replace the Fermi-golden-rule scattering rates shown in Fig. 1 by those calculated using the proper self-energy calculated self-consistently. In essence, the energy is no longer a single-value given by the momentum, but these two quantities are related by a probability function, the joint spectral density function, such as the Lorentzian approximation

$$P(E) = \frac{1}{\pi} [(E - p^2/2m - \Sigma_r)^2 + \Sigma_i^2]^{-1} \Sigma_i \ , \qquad (2)$$

where Σ is the proper self-energy (the imaginary part is the usual $h/\tau=\Gamma$). Equation (2) replaces the energy-conserving δ-function in the Fermi-golden rule, which in turn yields the self-energy Σ in the nearly free electron approximation. This expression is then solved self-consistently to give the new scattering rates, a procedure that has been carried out many times for semiconductors (Reich et al. 1983, Chang et al. 1983, and Fischetti and DiMaria 1985, Porod and Ferry 1985b). While most evaluate the expressions numerically, they can be solved in closed form in most cases. The largest changes are that sharp edges in the scattering rates, caused by the onset of new processes, are smoothed. In addition, the scattering rates are slightly enhanced in general, although strong peaks are greatly reduced back to the general background scattering rates. That is, the general effect is to reduce the effects of strong features in the scattering rates as a function of energy. These strong features relate closely to sharp features in the single particle density-of-states and it is these latter features which are strongly smoothed by equation (2).

The second problem in treating the transport in a fully quantum treatment is the transport equation. In principle, the motion of the carriers in the Monte Carlo process follows the classical trajectories. Fischetti and DiMaria (1985) used a Feynmann path integral to replace the normal Monte Carlo process, although quantum trajectories were randomly generated. On the other hand, Porod and Ferry (1985b) used the fact that in homogeneous electric fields the trajectories follow the semi-classical paths and extended the classical Monte Carlo approach. In both cases, the results did not differ greatly from that found with the semi-classical approach, as depicted by Fig. 2. Certainly, the values of the various coupling constants are not known well enough to be able to identify any significant changes in the transport.

A second quantum effect, whose role is totally unknown, is that of finite band-gap effects. Fischetti et al. (1985) point out that some band structure calculations suggest that the lowest conduction band in silicon dioxide has a finite width of the order of 5.0-5.5 eV. If this were the case, and no other bands were present, there would be a sharp drop in the density of states at this energy level. If so, it would be quite difficult for electrons to be accelerated above this energy, which would provide an energy bottle-neck for the distribution. Indeed, if there were no scattering at all, the average energy would approach the half-band value, but the velocity would be zero (Reich and Ferry, 1982). While it is unlikely that such a minimum in the density-of-states exists, it is an intriguing possibility and one that would make most of the discussion about details of the scattering processes irrelevant.

IMPACT IONIZATION

The dielectric strength of amorphous silicon dioxide has an important bearing on the performance and reliability of MOS structures, and consequently has been of interest for quite some time. Dielectric breakdown has generally been attributed to thermal breakdown or velocity runaway, with subsequent impact ionization in the latter case. Carrier multiplication has been treated by many authors and was applied to the case of silicon dioxide by the present author (Ferry, 1979). There, it was felt that velocity runaway allowed the carriers to accelerate to a sufficient energy that they would undergo an ionizing collision. However, this earlier model did not fit accurately the transport of the carriers themselves, as is now well known. Moreover, it is now quite widely believed that no impact ionization is observed experimentally for fields as high as 12 MV/cm (Fischetti et al., 1985).

To pursue this further, a model of the impact ionizing collision has been incorporated into the current ensemble Monte Carlo program. As Ridley (1987) has pointed out, most early theories of impact ionization have tended to assume that once the threshold for ionization was reached by a carrier, impact ionization was a very probably process. This is termed a "hard" threshold, and was used in the earlier studies (Ferry, 1979). However, there is a different version, which holds that the ionization is a "soft" process with a collision probability of the same form as other collision mechanisms. This was shown to be the case in Monte Carlo studies of narrow-gap semiconductors by Curby and Ferry (1973), and has recently been shown to be the case in moderate-gap semiconductors by Ridley (1987).

The lowest energy which an electron needs to create an electron-hole pair is determined by the conservation of energy and momentum during the scattering process. These conservation conditions were studied for general energy bands extensively by Anderson and Crowell (1972). This provides a threshold energy, given by

$$E_i = E_G[(1 + 2\mu)/(1 + \mu)] \quad , \tag{3}$$

where μ is the ratio of the electron mass to the hole mass. Thus, we are somewhat stymied by the uncertainty in the value of the latter parameter. By assuming a Coulomb interaction between the incident, high-energy electron and the bound electron, one can then calculate the scattering cross-section and relaxation time. In the present study, we use the form calculated by Curby and Ferry (1973) and by Ridley (1987). Once the scattering probability, as a function of energy, is known, this process can be incorporated into the Monte Carlo procedure. The number of ionizing collisions is monitored and the ionization rate α is calculated along with the other transport parameters. The ionization rate is plotted in Fig. 3, for two different values of the hole mass. It is seen, from this figure, that α rises rather slowly with electric field, regardless of the mass. Moreover, the absolute value of α is not large.

Traditionally, one expects impact ionization to lead to avalanche multiplication and breakdown when $\alpha L=1$; that is, when the product of the ionization and the transport length becomes unity. At 12 MV/cm, and a hole mass of 5.0m, α is only about 5000/cm, which requires an oxide thickness of 2 μm for breakdown by this process. Conversely, for an oxide thickness of 25 nm, we would require an ionization coefficient of 4 million per cm, which is more than two orders of magnitude larger than that found at this value of hole mass. It is more than an order of magnitude larger than observed with an infinite hole mass. These results seem to confirm the experimental conclusions that impact ionization by the electrons is not a significant factor in dielectric breakdown of silicon dioxide.

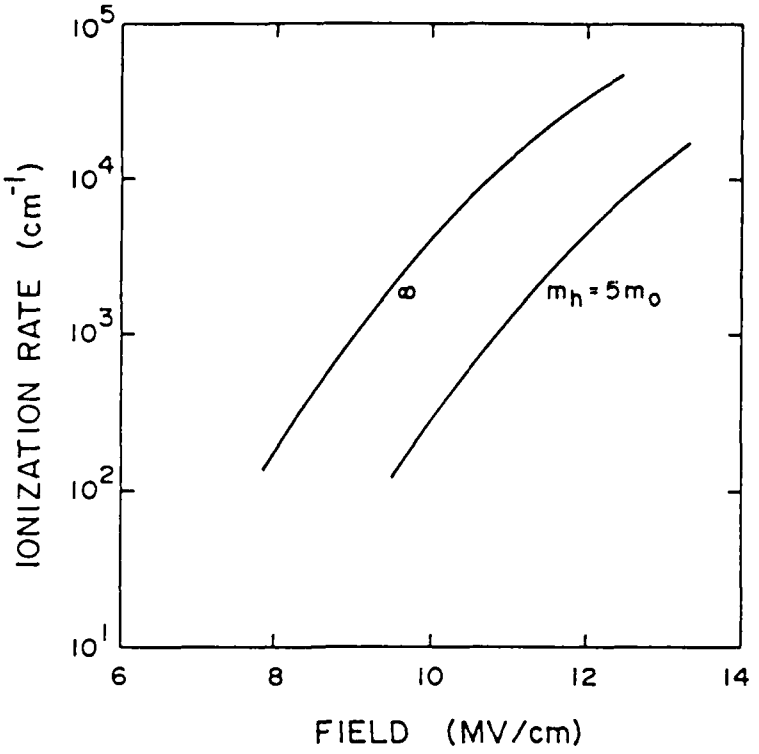

Fig. 3. The impact ionization coefficient for electron triggered ionization. The two curves are for different values of the hole mass.

CONCLUSIONS

Progress in the understanding of electron transport in silicon dioxide over the past several years has led to the conclusion that the electron distribution cannot be stabilized by interaction with the longitudinal polar optical phonon modes above 1.5-2.0 MV/cm, which is well below the levels expected earlier. For fields above this level, the mean carrier energy is found experimentally to rise to a level of 2-4 eV and to be stable at this value up to a field of 10 MV/cm. The only way in which this can be understood on the basis of interactions between the electrons and the lattice is for the presence of a high energy scattering process to provide a very large density of final states. Both acoustic umklapp and intervalley processes have been suggested for this extra scattering mechanism. However, our working knowledge of the properties of silicon dioxide really prevents us from drawing any definitive conclusions about which of the processes, if either, is responsible for the stabilization of the electron distribution.

Breakdown of the silicon dioxide has also been a subject of much interest for many decades. Early studies suggested that avalance breakdown, following impact ionization, was probably responsible, but this was not thought to be the case following recent experimental studies. In this present effort, the impact ionization collision was included in the Monte Carlo program, in order to investigate such an effect. The calculated ionization coefficient is far too small to realistically lead to avalanche breakdown in thin dielectric layers. Thus, we may conclude that breakdown of silicon dioxide is not likely to be due to impact ionization by electrons, at least for fields up to about 15-20 MV/cm.

The author would like to express his appreciation to M. Fischetti (IBM) and W. Porod (Notre Dame) for many helpful discussions. This work was supported in part by SDI/IST through the Office of Naval Research.

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