PHYSICAL REVIEW B VOLUME 45, NUMBER 3 15 JANUARY 1992-I

Acoustic-phonon runaway and impact ionization by hot electrons in silicon dioxide

D. Arnold, E. Cartier, and D. J. DiMaria

IBM Research Division, Thomas J. Watson Research Center, Yorktown Heights, New York 10598

(Received 11 October 1991)

We present model calculations for high-field electron transport in silicon dioxide based on recently measured energy-dependent electron-phonon scattering rates and impact ionization rates. We find a hot-electron runaway phenomenon in SiO_2, "acoustic-phonon runaway." This phenomenon occurs at electric fields exceeding 7 MV/cm, when acoustic-phonon scattering can no longer stabilize the hot electrons. A fraction of the electrons are accelerated in the electric field to energies high enough to generate electron-hole pairs by impact ionization. Simulated hole currents due to high-field impact ionization in SiO_2 gate oxides with thicknesses greater than 200 Å agree well with measured substrate hole currents in *n*-channel field-effect transistors. This suggests that these currents are due to holes generated by hot-electron impacts in the gate oxide.

Since the direct observation of strong electron heating in SiO_2 in the early 1980's, the concept of impact ionization has largely vanished from the literature of high-field studies in SiO_2. There are two reasons for this. First, DiMaria *et al.* have shown experimentally that the *average* energy of hot electrons does not exceed 6 eV even at fields as high as 10 MV/cm.[1] Such an energy stabilization has been theoretically explained by Fischetti in terms of a rapid increase of the acoustic-phonon scattering rate with increasing electron energy.[2] The discovery of this efficient scattering process at higher energies superseded older models, in which only longitudinal-optical (LO) phonons served to stabilize the electron energy distribution. Second, DiMaria and Stasiak[3] discovered that hot electrons with energies as low as 2 eV produce both positive and negative charge in the bulk and at the interfaces of metal-oxide-silicon (MOS) structures. This finding showed that positive charge buildup in the oxide (or at interfaces) is not in itself necessarily a signature of impact ionization. Theoretically, the problem of impact ionization was tackled by many authors.[3-7] Difficulties, however, arose from the fact that the energy dependences of neither the electron-phonon scattering rates nor the impact ionization rate were known and unambiguous predictions of impact ionization at high fields and its observable consequences could not be made. However, recently developed zero-field electron transmission techniques have now been used to perform direct measurements of the phonon scattering and impact ionization rates as a function of electron kinetic energy, including energies of the order of the band-gap energy and above.[8-11] This is an energy range crucial for calculations of electron-hole pair generation by impact ionization under high-field stress.

In this paper we investigate the implications of these measured electron-phonon scattering and impact ionization rates for high-field electron transport in SiO_2. We extend the model of Fischetti[2,12] so that the theoretical scattering rates agree with the measured rates. We solve the Boltzmann transport equation within this model via Monte Carlo integration. Our simulations reveal an electron runaway phenomenon—"acoustic-phonon runaway"—at electric fields above approximately 7 MV/cm. Acoustic-phonon runaway occurs when the electron scattering with acoustic phonons becomes too weak to stabilize the electron distribution at subband-gap energies and electrons accelerate to energies high enough to cause electron-hole pair generation by hot-electron impact. We show below that acoustic-phonon runaway is the controlling process for impact ionization in SiO_2. Quantities describing the *average* electron behavior are insensitive to the runaway phenomenon itself. However, strong experimental evidence for acoustic-phonon runaway can be found by measuring the hole current produced by high-field-induced impact ionization in the gate oxides of field effect transistors (FETs).

We describe the electron motion in our study by assuming a single valley band structure with the extended zone scheme.[2,13] The scattering rates for acoustic-phonon scattering and impact ionization used are in quantitative agreement with those measured by hot-electron transmission through thermal oxides.[8-11] At low energies, the measured acoustic-phonon scattering rates are in good agreement with values calculated within first-order time-dependent perturbation theory,[2,12] using a value of 6 eV for the acoustic deformation potential. This value has also been shown to account for the experimentally observed energy stabilization of the hot electrons at average energies of 2–6 eV at high electric fields.[1] The transmission experiments indicate a maximum in the acoustic rate below 8-eV kinetic energy and show a gradual decrease above 8 eV. The decrease at high energies is due either to a decrease in the density of states, or to a decrease in the deformation potential, or both. At the present time it is not possible to determine which of these phenomena is occurring due to a lack of reliable knowledge about the band structure at high energies. In our formalism the density of states increases at high energies in the manner prescribed by Fischetti,[2] but the deformation potential is set to zero for phonon wave numbers above $2.35 \times 10^{10} m^{-1}$. This choice is not based on a rigorous theory, and is therefore not unique; however, it forces good agreement between the model and the measured scattering rates. LO-phonon scattering is treated in the Fröhlich approximation using optical constants as given by Lynch.[14]

Finally, the impact ionization rates are obtained from direct measurements, and parametrized using the Keldysh formula.[15] We use a prefactor of 1.3×10^{15} sec^{-1} and set the threshold energy to the band gap, 9 eV. This parameter set reproduces the x-ray photoemission data.[8-11] It should be pointed out that this formula is not rigorously justified here, but is simply used as a convenient function to fit the measured ionization rate. This point is often overlooked in the semiconductor transport literature where the Keldysh formula has been routinely applied to complicated model band structures for which it is not strictly valid. In Fig. 1, we show a compiled summary of all scattering rates in terms of the total energy and momentum relaxation rates. The energy (momentum) relaxation rate is defined in the usual manner as the change in energy (momentum) with respect to time divided by energy (momentum). The interplay of these two relaxation rates allows a clear cut distinction between the various transport regimes in SiO_2 and the related runaway phenomenon. The rapid decrease of the energy relaxation rate above the energy of the dominant LO-phonon mode (153 meV) gives rise to the well-known phenomenon of "LO-phonon runaway." Upon entering the LO-phonon-runaway regime at fields above 2 MV/cm, the electrons gain more energy from the field than they lose to the lattice via LO-phonon emission and they are rapidly accelerated until they reach energies in excess of 2 eV. At energies of 3–6 eV, the momentum relaxation rate increases sharply, due to quasielastic, isotropic (acoustic) scattering, while the energy relaxation rate stays approximately constant because of the small energies involved in acoustic scattering. In this dispersive transport regime, large-angle scattering strongly enhances the path length in the solid compared to a straight flight in the field direction and therefore the number of emitted LO phonons rapidly increases with this increasing momentum relaxation rate. The electron energy distribution is again stabilized at average energies of 2–6 eV over a wide range of applied electric fields.[1] This stabilization process cannot hold for arbitrarily high fields, however, since the momentum relaxation rate is now known to decrease above about 6 eV, while the energy relaxation rate is fairly constant up to the threshold for impact ionization ($\simeq$9 eV). Runaway from the acoustic phonons is expected at even higher fields, leading to impact ionization and a restabilization of the energy distribution by the strong energy relaxation involved in this process.

Porod and Ferry have reported an alternative model which includes satellite valleys in the band-structure model and emphasizes intervalley scattering.[16] More research, both experimental and theoretical, is required to determine which model, or combination of models, is most appropriate. However, a version of the multivalley model which quantitatively reproduces the x-ray photoemission[8-11] data will likely yield energy and momentum scattering rates qualitatively similar to those in Fig. 1. In this case a phonon runaway phenomenon at energies of a few electron volts will still be observed, even if the relevant scattering mechanism is intervalley scattering.

In order to quantify this electron runaway phenomenon, we have calculated transient and steady-state electron energy distributions for oxide films with thicknesses up to 1000 Å and applied electric fields of up to 15 MV/cm. Typical simulated electron energy distributions are shown in Fig. 2. These distributions were obtained by averaging 10000 sample electrons over a 500-Å-thick film, which yields an adequate representation of steady-state energy distributions. The figure illustrates rapidly increasing high-energy tails extending well beyond band-gap energies with increasing electric-field strength. Above 7 MV/cm, acoustic scattering is too weak to stabilize the energy distribution below the maximum in the momentum relaxation rate, and the electrons escape to energies high enough to cause impact ionization. However, acoustic runaway is largely masked by the high-energy losses involved in impact ionization. An electron initiating an impact ionization event gives up most of its kinetic energy and becomes part of the distribution in the dispersive transport regime. Thus, there is a steady stream of elec-

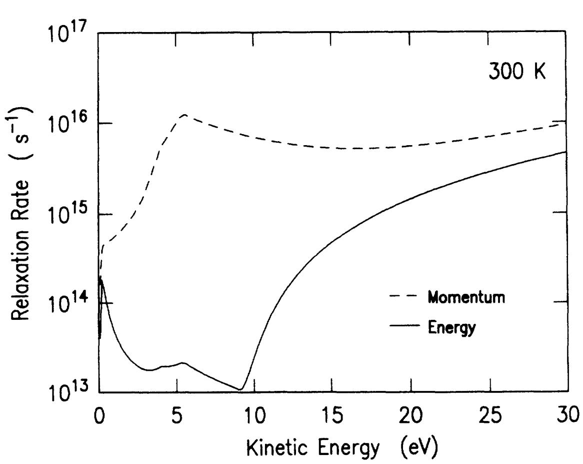

FIG. 1. Hot-electron energy (solid line) and momentum (dashed line) relaxation rates in SiO_2 vs electron energy at room temperature.

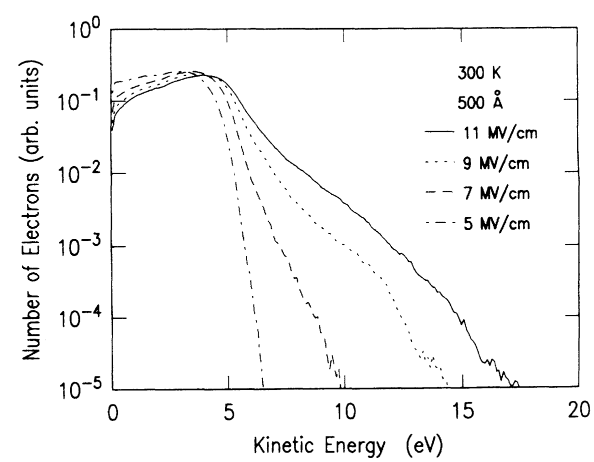

FIG. 2. Simulated electron energy distributions in SiO_2 using the rates shown in Fig. 1. The distributions are averaged over an oxide thickness of 500 Å for oxide fields between 5 and 11 MV/cm.

trons to energies above 9 eV even though most of the electrons at any given time are below this energy. Only because impact ionization has a soft threshold do the high-energy tails extend beyond band-gap energies. Such energy tails in the electron distribution extending to energies of 20 eV have been observed using vacuum emission techniques.[17] The strong energy relaxation accompanying impact ionization (see Fig. 1) thus renders quantities describing the average behavior of the hot electrons insensitive to acoustic runaway. For example, average energies calculated from the simulated distributions do not show any obvious change due to acoustic runaway. This is consistent with the measured average electron energies up to fields of 10 MV/cm.[1]

We have performed measurements of substrate hole currents in n-channel silicon field effect transistors which provide a direct observation of hole generation by hot-electron impact in SiO_2 after acoustic runaway. In these measurements, a positive voltage is applied to the gate with respect to the FET channel. There is a negative built-in potential at the substrate with respect to the channel due to the induced p-n junction. Electrons are injected into the SiO_2 gate from the channel via Fowler-Nordheim tunneling. These electrons are supplied by the source and drain contacts which are both grounded. When, as described above, the oxide electric field exceeds about 7 MV/cm, impact ionization transpires in the oxide. The holes produced by impact ionization move towards the silicon substrate and are collected as a Si substrate current and thus provide a measure for the number of impact ionization events in the gate oxide. The ratio of the substrate and the channel current, $\alpha = I_s/I_{ch}$, is then simply the number of impact ionization events in the gate per injected electron, provided that all holes are collected and no other mechanism contributes to the substrate current. In Fig. 3, we show measured current ratios in FETs with oxide thicknesses ranging from 245 to 957 Å. Our data are consistent with similar measurements reported earlier by a number of researchers.[18–24] In the thickness range

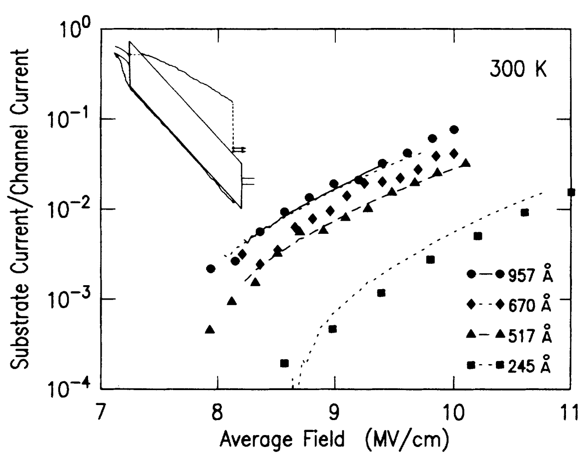

FIG. 3. Measured (curves) and calculated (symbols) values for the ratio of the substrate current to the channel current in n-channel FET as a function of oxide field. Results are shown for oxide thicknesses of 245, 517, 670, and 957 Å.

shown in Fig. 3, α depends only on the average field in the gate oxide and is relatively insensitive to the degree of interface and bulk charge buildup or to the fabrication conditions of the FETs. Two major sources of spurious hole currents are generation-recombination centers in the silicon and light emission from hot-electron relaxation in the gate which in turn may lead to electron-hole pair generation in the substrate. We have measured these contributions independently. They are found to be small compared to the total hole current, except for the 245-Å sample. A constant contribution of 10^{-3} due to the above spurious sources was subtracted from α.

We have calculated the number of holes generated by impact ionization per electron injected into SiO_2 gate insulators using the Monte Carlo method described above. The comparison of calculated (symbols) and measured (lines) current ratios in Fig. 3 shows excellent, and before this work unexpected agreement between the two. Once an electron escapes from the region of strong acoustic scattering to energies of the order of the band gap, it is rapidly accelerated to energies sufficient to create an electron-hole pair. This renders the calculation more sensitive to the absolute magnitude of the acoustic rate than to the impact ionization rate itself. It is this acceleration to the threshold energy for impact ionization which is the rate limiting process, not the rate of impact ionization once the threshold energy has been attained. Our model not only predicts good absolute current ratios in the steady-state regime, but it also yields a thickness dependence which is consistent with the experimental data. At fields above 7 MV/cm, an oxide thickness of about 300 Å is required in order to allow the electron distribution to evolve from the injected Maxwellian into the steady-state energy distribution with fully developed high-energy tails. Due to this heating transient, the hole current is found to turn on rapidly over an initial thickness range of about 300 Å. This trend is shown by the experimental data in Fig. 3. Only at thicknesses above about 500 Å does α scale with oxide thickness t_{ox}, as $\alpha = 2^{\beta t_{ox}} - 1$, where $\beta(F)$ is the field-dependent impact ionization coefficient. It was not previously clear that the measured thickness dependence is consistent with impact ionization. Our calculations now show that the rapid onset of the hole current with increasing film thickness (at a constant field) can be quantitatively attributed to the spatial transient in the electron heating.

The calculated hole currents are very sensitive to the chosen absolute values of the momentum relaxation rate above 6 eV. Therefore, the limited accuracy of the zero-field transport experiments[8–11] leaves the calculated current ratios uncertain within about a factor of 2. The uncertainties in the calculated current ratios due to the experimental uncertainties of the impact ionization rate are less critical. This is a consequence of the nature of the rate limiting step for hole production, which in the runaway scenario is the acceleration of the hot electrons out of the dispersive transport regime at around 6 eV of kinetic energy up to the threshold energy. For this reason, comparison of the calculated and measured substrate hole currents provides a sensitive means to fine tune the acoustic-phonon scattering rates in our model.

In conclusion, we have shown that the recently reported values for the acoustic scattering rates and impact ionization rates[8–11] imply the existence of a quantitatively high-field-transport phenomenon in SiO_2, acoustic-phonon runaway. This phenomenon is shown to be the controlling mechanism for impact ionization. Strong evidence for acoustic-phonon runaway was obtained from the quantitative prediction of substrate hole currents due to high-field impact ionization in gate oxides of *n*-channel FETs.

The authors would like to acknowledge helpful discussions with M. V. Fischetti, F. R. McFeely, and P. Price. The assistance of S. Laux and G. McNiven with computing was invaluable.

[1]D. J. DiMaria, T. N. Theis, J. R. Kirtley, F. L. Pasavento, D. W. Dong, and S. D. Brorson, J. Appl. Phys. **57**, 1214 (1985).

[2]M. V. Fischetti, Phys. Rev. Lett. **53**, 1755 (1984).

[3]D. J. DiMaria and J. W. Stasiak, J. Appl. Phys. **65**, 2342 (1989).

[4]P. Solomon and N. Klein, Solid State Commun. **17**, 1397 (1975).

[5]R. C. Hughes, Solid-State Electronics **21**, 251 (1978).

[6]D. K. Ferry, J. Appl. Phys. **50**, 1422 (1979).

[7]S. Jones, P. Braunlich, R. Casper, X. Shen, and P. Kelly, Opt. Eng. **28**, 1039 (1989).

[8]E. Cartier and P. Pfluger, Phys. Scr. **T23**, 235 (1988).

[9]F. R. McFeely, E. Cartier, J. A. Yarmoff, and S. A. Joyce, Phys. Rev. B **42**, 5191 (1990).

[10]F. R. McFeely, E. Cartier, L. J. Terminello, A. Santoni, and M. V. Fischetti, Phys. Rev. Lett. **65**, 1937 (1990).

[11]E. Cartier and F. R. McFeely, Phys. Rev. B **44**, 10689 (1991).

[12]M. V. Fischetti, D. J. DiMaria, S. D. Brorson, T. N. Theis, and J. R. Kirtley, Phys. Rev. B **31**, 8124 (1985).

[13]M. Sparks, D. L. Mills, T. Hostein, A. A. Mardudin, L. J. Sham, E. Loh, Jr., and D. F. King, Phys. Rev. B **24**, 3519 (1981).

[14]W. T. Lynch, J. Appl. Phys. **43**, 3274 (1972).

[15]B. K. Ridley, *Quantum Processes in Semiconductors* (Clarendon, Oxford, 1988).

[16]W. Porod and D. K. Ferry, Phys. Rev. Lett. **54**, 1189 (1985).

[17]D. J. DiMaria and M. V. Fischetti, J. Appl. Phys. **64**, 4683 (1988).

[18]Z. A. Weinberg, W. C. Johnson, and M. A. Lampert, Appl. Phys. Lett. **25**, 42 (1974).

[19]A. S. Ginovkev, V. A. Gritsenkor, and S. P. Sinitsa, Phys. Status Solidi A **26**, 489 (1974).

[20]B. Eitan and A. Kolodny, Appl. Phys. Lett. **43**, 106 (1983).

[21]L. D. Yau, F. T. Liou, and S. Chen, IEEE Electron Device Lett. **EDL-4**, 261 (1983).

[22]D. J. DiMaria, D. W. Dong, C. Falcony, T. N. Theis, J. R. Kirtley, J. C. Tsang, D. R. Young, and F. L. Pasavento, J. Appl. Phys. **54**, 5801 (1983).

[23]Z. A. Weinberg and M. V. Fischetti, J. Appl. Phys. **57**, 443 (1985).

[24]Z. A. Weinberg, M. V. Fischetti, and Y. Nissan-Cohen, J. Appl. Phys. **59**, 824 (1986).