Monte Carlo Solution to the Problem of High-Field Electron Heating in SiO_2

Massimo V. Fischetti
IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598
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By use of a Monte Carlo technique, it is shown that high-field electron transport in the SiO_2 conduction band is controlled by LO-phonon scattering for fields below 3×10^6 V/cm and by nonpolar scattering with acoustic phonons at higher fields. This accounts for recent experimental results indicating that an energy-loss mechanism, previously neglected, is effective at high fields.

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Starting with the pioneering work of Thornber and Feynman,[1] the electron transport in polar insulators has been treated theoretically under the assumption that the longitudinal-optical (LO) phonons are the only significant scatterers. Application[2-4] of this idea to SiO_2 has led to the conclusion that the LO phonons are able to maintain the average electron energy below the energy of the dominant polar mode ($\simeq 0.15$ eV) for field strengths as high as 7×10^6 to 10×10^6 V/cm. This conclusion depended mainly on a very short mean free path ($\lesssim 0.2$ nm) for the electron-phonon interaction. Only at higher fields would the electrons begin to gain an appreciable energy and this would occur in an uncontrolled regime of "velocity runaway," eventually leading to impact ionization and breakdown.[5]

Some difficulties with this picture arise from the fact that much longer mean free paths (2 to 4 nm) must be assumed to explain the efficiency of internal photoemission,[6] the observation of resonant tunneling in thin SiO_2 layers,[7] and the emission of electrons from SiO_2 to the vacuum.[8] This suggests that the theoretical results mentioned above could be affected by an overestimation of the polar electron-phonon interaction in a weakly polar material such as SiO_2. In addition, serious problems with the "LO-phonon–based" picture were recently brought to light by Fitting and Friemann.[4] Employing a Monte Carlo simulation, they showed that the LO phonons cannot prevent the electrons from "running away" towards higher and higher energies even at fields as low as 1.5×10^6 V/cm, that is, about 1 order of magnitude below the observed breakdown fields. These predictions were confirmed experimentally by the recent work of Theis and co-workers.[9,10] By employing three different experimental techniques, Theis *et al.*[9] and DiMaria *et al.*[10] observed a significant electron heating at fields as low as 5×10^6 V/cm, without destructive breakdown occurring. At higher fields, up to 1.2×10^7 V/cm, the average electron energy increased, but no runaway was observed. The conclusion was that another scattering mechanism took over after the LO-phonon uncontrolled runaway had occurred.

In search for such a mechanism, attention was focused on the scattering with acoustic phonons. Indeed, as the elctrons reach the threshold for emission of acoustic phonons via umklapp (U) processes, which can occur at energies $w \gtrsim w_{BZ}/2$ (w_{BZ} being the energy of the electrons at the Brillouin-zone boundary), the probability of having Bragg reflections increases and it becomes harder and harder for the carriers to gain more energy from the field. These ideas had already been applied to alkali halides,[11] but were left as simple proposals in the case of SiO_2.[12]

The scope of this Letter is to pursue this idea and show that indeed the properties of the electron transport in SiO_2 can be understood *only if proper account is made for the scattering with the nonpolar lattice vibrations.* A Monte Carlo technique—similar to the one used by Fitting and Friemann[4] and Baidyaroy *et al.*[13]— has been employed to solve the transport equation for electrons in the SiO_2 conduction band *including scattering with the nonpolar modes via U and normal (N) processes as well as with the polar modes.*

The two significant LO-phonon branches (0.063 and 0.153 eV) have been treated with the usual Fröhlich Hamiltonian formalism.[14] The scattering rate $1/\tau$ resulting from the nonpolar coupling to the acoustic phonons has been calculated in the parabolic-band approximation, following Sparks *et al.*[11] from the expression[15,16]

$$\frac{1}{\tau^{\pm}(\vec{k})} = \sum_{\alpha} \frac{m^*}{4\pi M N_c \hbar^2 k} \int_0^{q_{\max}} dq \frac{q^3}{\omega_{\alpha}(\vec{q})} |S_{\alpha}(\vec{q})|^2 [n_{\alpha}(\vec{q}) + \tfrac{1}{2} \pm \tfrac{1}{2}], \tag{1}$$

for emission (+) or absorption (−) of one phonon. The sum extends over the branches α of the nonpolar modes, m^* is the electron effective mass, N_c is the density of primitive cells, M is the mass of a primitive cell for small phonon momenta q, or the mass of the heaviest constituent of the cell as q approaches k_{BZ}, the boundary of the first Brillouin zone (BZ), k is the electron wave vector, and the $n_\alpha(\vec{q})$'s are the Bose factors of the various phonon branches. The phonon dispersion has been assumed to be $\hbar c_S q$ for small q, c_S being the SiO_2 sound velocity, and $\hbar c_S k_{BZ}$ as $q \gtrsim k_{BZ}$. Finally, $q_{max} = 2k \pm 2m^* c_S/\hbar$ is the maximum momentum an emitted (−) or absorbed (+) phonon can have. No distinction has been made between transverse and longitudinal modes and the label α will be dropped in the following.

The matrix element $S(\vec{q})$ has been assumed to be independent of the momentum transfer. For low-frequency phonons, one can assume that $|S(\vec{q})| \simeq C_1$, the deformation potential.[17] At large q, an expression for S in terms of a measurable quantity is given by[16]

$$|S(\vec{q})|^2 \simeq (\pi\hbar^4 N^2/m^{*2})\sigma, \qquad (2)$$

where σ is the integrated cross section related to the form factor of the lattice and N is the atomic density.

The choice of the values of the parameters to be employed in the numerical simulation is a major issue. It was found that w_{BZ} is the critical parameter fixing the average electron energies at various fields. It has been obtained by considering a spherical BZ with volume equal to the volume of the BZ of α quartz,[18] and assuming an electron effective mass of $0.5 m_{free}$ at the bottom of the SiO_2 conduction band. The value obtained in this way, 5.5 eV, is consistent with the band structure calculated by Chelikowsky and Schlüter.[19] The parameter σ has been obtained by assuming that the large oxygen ion is mostly effective in scattering electrons. Its integrated cross section, 3.5×10^{-15} cm^2,[11] has been rescaled by the average, dynamic effective charge of oxygen in SiO_2 ($\simeq 1.1e$, as given by Pantelides and Harrison[20]) to account for the large covalence of the Si-O bond in SiO_2. Inserting the density of the oxygen ions in Eq. (2), one obtains $|S(\vec{q})| \simeq 3.5$ eV. The same value for $S(\vec{q})$ has been employed over the whole energy range, in the absence of any experimental information about C_1. This is not a critical issue, since the acoustic phonons play a negligible role in the scattering at low energies (small q). The effective mass m^* has been set equal to the free-electron mass in the high energy range of interest here. Finally, the SiO_2 sound velocity has been obtained from an average of the longitudinal (c_L) and transverse (c_T) velocities in SiO_2 (from Ref. 21) according to $3/c_S \simeq 2/c_T + 1/c_L$.

Results for a finite value of the temperature could be obtained with relatively reasonable computing times only by using the high-temperature expansion for the Bose factor in Eq. (1) in the low-energy range.

In order to perform the numerical simulation, the low-energy ($w < w_{BZ}/2$) and the high-energy ($w > w_{BZ}$) limits of Eq. (1) have been algebraically interpolated. The resulting scattering rates at 298 K are shown in Fig. 1 as functions of the electron energy. The electrons have been assumed to enter the SiO_2 with zero energy. In case of N processes ($q < k_{BZ}$), the polar scattering angle has been obtained from energy and momentum conservation after a random choice of the momentum q with probability weighted by Eq. (1), according to the Metropolis-Ulam algorithm.[22] The polar angle has been randomly chosen in the case of U processes, also in view of the amorphous structure of thermally grown SiO_2.

The simulation program was written in Fortran 77 and run on an IBM 3081 computer. Typically, a satisfactory convergence for the average electron energies and energy distributions was obtained after the "injection" of 500 to 1000 electrons.

The main result of this work is summarized in Fig. 2. The average electron energy at 298 K is shown as a function of the electric field. Comparison is made with the experimental data of Refs. 9 and 10, plotted as functions of the anode field. A satisfactory agreement is observed *which could not be obtained when only scattering with the LO phonons*

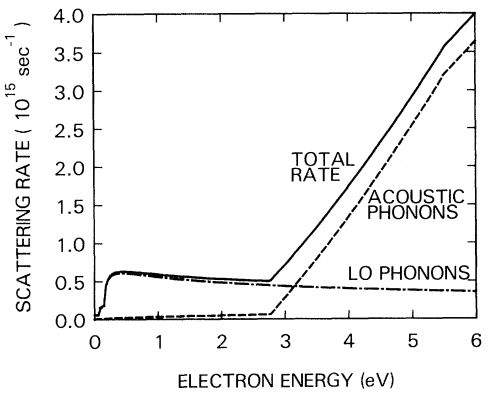

FIG. 1. Total (emission and absorption) scattering rates as functions of the electron energy at 298 K.

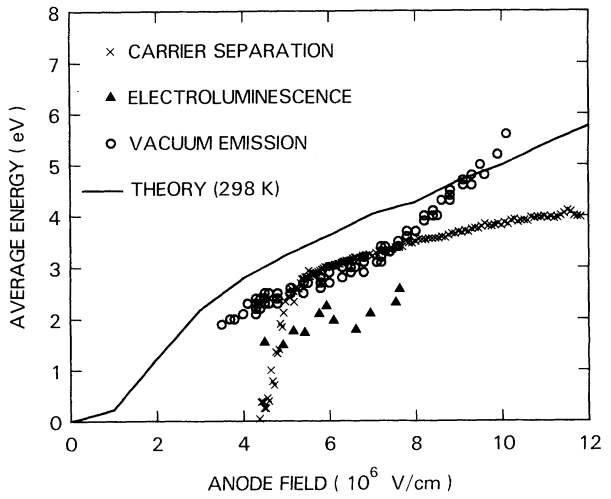

FIG. 2. The average electron energy as a function of the electric field. A comparison is made between the results of the Monte Carlo simulation at 298 K (solid line) and the results of the experiments described in Refs. 9 and 10.

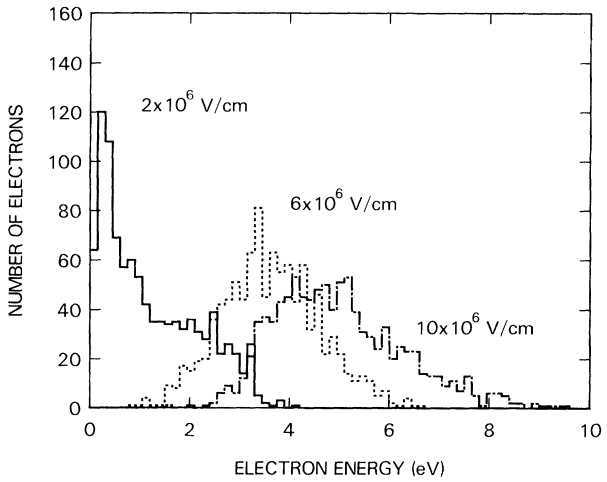

FIG. 3. Energy distributions of the hot electrons at various field strengths. The results refer to simulations performed with the assumption of an oxide thickness of 50 nm.

was considered.

The basic picture can be understood as follows. At fields below $F_{th} \approx 1.5 \times 10^6$ V/cm, the LO phonons control the energy losses. Above this field, an uncontrolled velocity runaway would occur if the acoustic phonons did not take over. The transition between the LO- and acoustic-phonon–dominated regime is seen in Fig. 2 in the sudden increase of the average energy above 1×10^6 V/cm. In the acoustic-phonon–controlled regime, the electrons have an increasing probability of suffering large-angle collisions (large momentum transfer) via nonpolar interactions as their energy increases. It is obvious that the inclusion of U processes is a key element in this picture, since their large-angle scattering increases the length of the electron trajectories. This allows more and more energy to be lost also to the LO phonons, which still absorb a non-negligible fraction of the electron energy. As a result, the electron distribution is stable even at very high fields, the average energy increasing with the field approximately as $e\lambda F_{0x}$, F_{0x} being the electric field and λ a characteristic length taking the value of ≈ 3.5 nm at 298 K.

A few electron energy distributions at 298 K and at various field strengths are shown in Fig. 3. Because of a limited amount of computing time —which will be extended in the future—the poor statistics in the high-energy "tail" of the histograms makes it premature to draw any conclusion about the fractions of carriers which could suffer inverse Auger scattering (impact ionization) at high fields. It should also be remembered that for high electron energies the nonparabolicity of the SiO_2 conduction band and "collision-broadening" effects, due to the uncertainty of the electron energy between collisions, are likely to modify dramatically the properties of electron transport.[23]

The average electron energy and energy distributions are found to reach steady-state conditions (field thermalization) after a distance of about 3 to 7 nm, decreasing with increasing field. This implies that a comparison between the numerical results and the experimental data of Refs. 9 and 10 must be made at a given anode field, as has been done in Fig. 2.

Finally, the "injection" of electrons with nonzero energy has been simulated. Again, a field-thermalization distance of less than 7 nm has been found. The probability that one electron with initial energy between 0 and 1 eV suffers no collision in the first 2 nm is significant ($\gtrsim 15\%$). This may account for the observations of large internal-photoemission efficiencies and of resonant tunneling in 4.6-nm-thick SiO_2 layers.[7]

In conclusion, it has been shown that the interaction with the nonpolar phonons, in particular via umklapp processes, is a key element needed to explain the observed properties of electron transport in SiO_2.[9,10]

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