Monte Carlo Study of High-Energy Electrons in Silicon Dioxide

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A Monte Carlo study of high-field electronic transport in silicon dioxide is undertaken. Contrary to previous theoretical studies, we do not model the electronic structure by a single free-electron-like band. Our model accounts for a set of satellite valleys which contribute density of states needed for effective scattering at a few electronvolts. We find that the electronic distribution is stable for fields on the order of 10 MV/cm.

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The study of high-field electronic transport in silicon dioxide has been the subject of numerous investigations.[1-4] This interest stems from the importance of SiO_2 as an insulator for microelectronics. For ultralarge-scale integration, fields in the insulator are on the order of a few megavolts per centimeter and thus close to electrical breakdown. For carrier transport under these high fields, the scattering by polar optical phonons was believed to be the dominant scattering mechanism.[2-4] Through the emission of optical phonons, electrons can lose the energy which they gain in the electric field. It was argued that this loss of energy would keep the carriers from continuously gaining energy in the field (polar runaway) and that the electronic distribution was stabilized at an average electron energy below the phonon energy.

Over the last few years, this belief was challenged by the finds of experimental as well as theoretical studies. By use of the Monte Carlo technique,[5] it was shown that LO (longitudinal optical) phonons by themselves cannot prevent polar runaway even for comparatively low fields. In these calculations, the onset of polar runaway was reported for a field of 1.5 MV/cm, which is 1 order of magnitude lower than the experimentally observed breakdown field. Even more recently, experimental studies[6] for fields of several megavolts per centimeter have shown that the electronic distribution is stable and that the average energy is on the order of a few electronvolts and thus considerably larger than the energy of polar optical phonons. These findings imply that optical phonons are not the dominant mechanism of energy loss at these high fields. Consequently, there has to be some additional scattering mechanism which keeps the electrons from polar runaway and which stabilizes their average energy at a few electronvolts.

Very recently, a candidate for such a mechanism has been proposed.[7] It was suggested that acoustic umklapp (U) scattering becomes very efficient at high energies. As electrons reach the threshold for the emission of acoustic U processes, the probability of having Bragg reflections increases, which keeps the carriers from gaining more energy from the electric field. On the basis of this idea, a Monte Carlo study was undertaken and it was reported that these additional scattering processes keep the electronic distribution stable at average energies of several electronvolts.[7] However, at these energies, the details of the band structure must be considered, and this has been ignored until now. In this paper, we show that the existence of subsidiary valleys of the conduction band are important in the understanding of transport in SiO_2.

A key to an understanding of electronic transport is the knowledge of the electronic structure. In all theoretical transport studies so far, the electronic structure of SiO_2 was assumed to be free-electron-like with an effective mass ranging from $0.5m_0$ to $1.5m_0$. In contrast to that, the electronic band structure looks only free-electron-like for low energies. For energies of a few electronvolts, the density of states looks significantly different, and it is clear from theoretical studies that additional conduction-band valleys must be considered.[8-11]

It has been argued that the general features of the electronic structure for various crystalline modifications of SiO_2 are quite similar despite their different crystal structures. Using the tight-binding technique, calculations of the density of states for α-quartz[8] (hexagonal) and β-cristobalite[9] (zinc blende) show a peak at energies close to 2 eV above the conduction-band edge. On the other hand, calculations using the pseudopotential method[10] show that these valleys lie some 3.5 eV above the conduction-band minimum in α-quartz. The most striking feature is an almost flat dispersion along the H-to-A line in k space for α-quartz. This general behavior is also observed for amorphous SiO_2. It is clear that an increased density of states, arising from the presence of the satellite valleys, should lead to an increase of the scattering probability for electrons at these energies, and that it has to be included in a proper model.

We perform a Monte Carlo study of high-field transport in SiO_2 based upon this idea. The usual acoustic and LO-phonon scattering mechanisms are included and, in addition, we also model the effect of higher bands by means of satellite valleys. Of crucial importance is the choice of parameters in the numerical simulation. We will discuss this in some detail below.

Our strategy is to choose the parameters for the central valley so that low-field velocity data are reproduced. We model the band structure of SiO_2 by a central valley and a set of high-energy equivalent satellite valleys. In analogy to α-quartz, we assume twelve partial (two total) valleys which correspond to minima at the H point in k space. For simplicity, each valley by itself is assumed to be parabolic. The effective mass for the satellite valleys is estimated from the intensity of the density-of-states peak to be $m_2^* = 1.5 m_0$; variations from this value are discussed.

Little is known about the phonon spectrum of SiO_2, which makes the choice of phonons for intervalley scattering difficult. Data for the phonon density of states indicate three strong peaks.[11] Two correspond to polar optical phonons with energies of 0.153 and 0.063 eV, respectively. The third peak corresponds to an energy of 0.1 eV. We choose this phonon for intervalley scattering. The scattering probability for the Monte Carlo simulation is modeled analogous to nonpolar optical scattering[12] with a standard value of the deformation potential of 10^9 eV/cm. The scattering between equivalent satellite valleys is modeled in the same way. For scattering in each valley, the intravalley acoustic deformation potential has previously been found[4,12] to range between 5 and 25 eV. Here, we adopt a value of 25. For polar optical scattering within each valley, two dominant modes have been identified before. The high-energy polar LO phonon with energy of 0.153 eV has a coupling strength of $\epsilon_\infty^{-1} - \epsilon_0^{-1} = 0.143$. A second strong LO phonon exists at an energy of 0.063 eV and has a coupling parameter of $\epsilon_{\rm int}^{-1} - \epsilon_0^{-1} = 0.063$, where $\epsilon_{\rm int}$ is the dielectric constant for energies between the two LO modes.

The Monte Carlo procedure used here is standard and has been described in the literature.[5,7] We follow the trajectories of an ensemble of electrons and perform averages over this ensemble. Satisfactory convergence was obtained for an ensemble of 1000 electrons. The initial energies and momenta are determined from an equilibrium Maxwell-Boltzmann distribution; a temperature of $T = 300$ K has been used throughout.

In Fig. 1, we show a comparison of experimental low-field drift-velocity data[13] and the drift velocity calculated here. We find that, for fields up to about 2 MV/cm, all electrons remain in the central valley. Correspondingly, the fit to the low-field data is only determined by the parameters of the central valley. The drift velocity depends sensitively upon the choice of the effective mass and the acoustic deformation potential. A good fit, which is shown in Fig. 1 by the solid line, is obtained for a central-valley effective mass of $m_1^* = 0.5 m_0$ and a deformation potential of 25 eV. The same mass has been used by Fischetti[7] and has been estimated from band-structure calculations,[8] and this deformation potential has previously been used for transport analysis.[4] No negative differential mobility was observed for any field.

In Fig. 2, we show a comparison of experimental values for average electron energies at high fields and compare them to our results. Two different values for the separation between central and satellite valleys are used. Curve a corresponds to a separation of 1.75 eV; curve b is for 3.0 eV. The dependence of these results on the effective mass in the satellite valleys is shown in Fig. 3 for a valley separation of 1.75 eV. We find a gradual increase of the energy with electric field to a saturation value which is largely determined by the valley separation. The fraction of electrons in the satellite valley is typically 50% at a field of 10 MV/cm. These results have been found to be insensitive to the

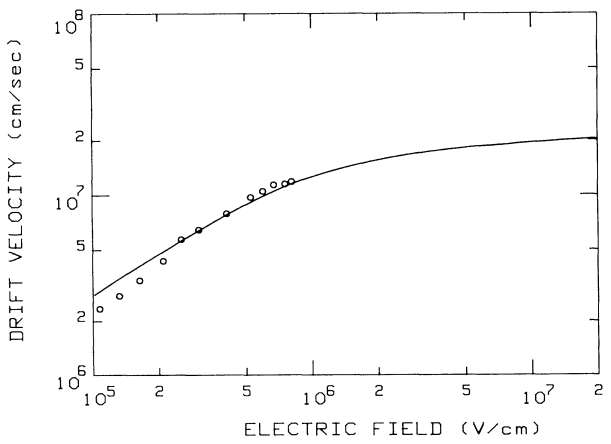

FIG. 1. Comparison of experimental data (Ref. 13) (circles) and the result of the Monte Carlo study (solid line) for $m_1^* = 0.5 m_0$ and an acoustic deformation potential 25 eV.

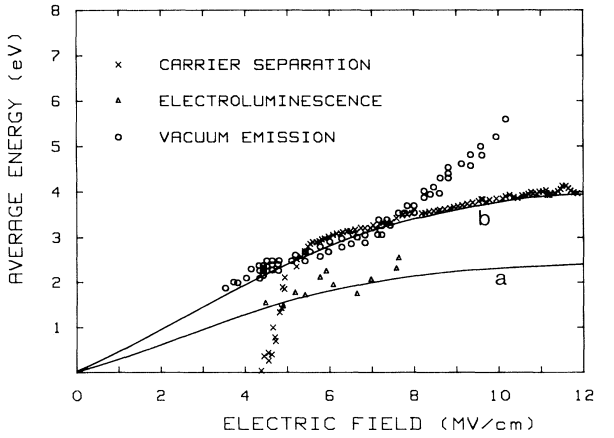

FIG. 2. Dependence of the average energy on the valley separation. Curve a is for a separation of 1.75 eV; curve b is for 3 eV; $m_2^* = 1.5 m_0$ is used. The experimental data are from Refs. 6 and 7.

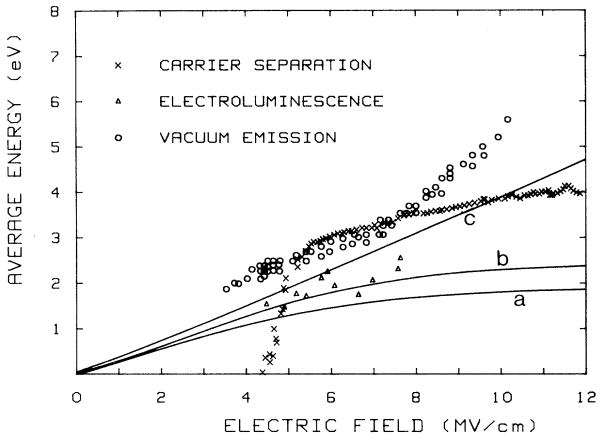

FIG. 3. Dependence of the average energy on the effective mass in the satellite valleys. For curve *a*, $m_2^* = 2.0m_0$; for curve *b*, $m_2^* = 1.5m_0$; and for curve *c*, $m_2^* = 1.0m_0$; a valley separation of 1.75 eV is used.

energy of the intervalley phonon.

The essence of our results is therefore that the inclusion of satellite valleys, which provide additional scattering mechanisms at high energies, can prevent polar runaway and can stabilize the electronic distribution at average energies of a few electronvolts. These qualitative conclusions are largely independent of the choice of parameters used for the simulation. Therefore, we expect these qualitative conclusions to hold true even if better data become available for the details of scattering at high energies. Detailed comparison with experimental data is hampered not only by the spread in experimental results, but by the lack of agreement on the details of the satellite valleys.

We also want to address the problem of using a semiclassical Monte Carlo approach for these extremely high fields. For these short collision times, quantum effects, such as the intracollisional field effect[4] and implications of the uncertainty principle, should become important. Indeed, it has been shown[14] that these effects become noticeable for fields of about 10 MV/cm. We expect that in the very-high-field regime, our results are not quantitative with this semiclassical approach. However, we expect the qualitative conclusions to hold true, and a study of quantum effects is planned for the future.

In conclusion, we find that the incorporation of subsidiary conduction-band minima, which correspond to peaks in the density of states at energies of a few electronvolts above the conduction-band edge, is able to stabilize the electronic distribution at fields on the order of 10 MV/cm. The effect of these satellite valleys on the transport was investigated with a Monte Carlo study and, using the same set of parameters, we were able to gain agreement with both low-field velocity data and carrier energy data at high electric fields.

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