SIMULATION OF SEMICONDUCTOR DEVICES AND PROCESSES Vol. 5
Edited by S. Selberherr, H. Stippel, E. Strasser - September 1993

Electron Transport in Silicon Dioxide at Intermediate and High Electric Fields

M. Hackel, H. Kosina, and S. Selberherr

Institute for Microelectronics, TU Vienna
Gußhausstraße 27-29, A-1040 Wien, AUSTRIA

Abstract

A semiclassical Monte Carlo technique is employed to simulate the steady-state electron transport in silicon dioxide at intermediate and high electric fields. The electronic band-structure is modelled by a single parabolic, by a single nonparabolic as well as an isotropic four-band model. We find that the electronic behavior of silicon dioxide is mainly influenced by a single nonparabolic conduction-band.

1. Introduction

In the seventies and the early eighties the standard picture of electron transport in insulators assumed only one scattering process to be dominant, the longitudinal polar optical phonons due to the ionic character of Silicon dioxide (SiO_2) [1],[2],[3]. In the mid eighties new experimental data predicted breakdown fields higher than calculated in theoretical studies. Ridley [4] supposed a new scattering mechanism to prevent polar runaway, namely nonpolar acoustic phonons. Sparks *et al.* [5] derived a mathematical formulation of this process. Despite of the ionic character of the electronic bonds in alkali halides, nonpolar acoustic phonons stabilize the electronic distribution and increase the electrical breakdown-field. A theoretical investigation for SiO_2 was first made by Fischetti [6] and it was found that collisions between electrons and nonpolar acoustic phonons indeed have strong impact on the electronic behavior of oxides. The data of several experiments could be well reproduced [7].

2. The Physical Model

Insulators partially have ionic character, thus electrons lose energy to the lattice in form of polar longitudinal optical (LO) phonons. Electrons in SiO_2 strongly interact with two LO phonon modes via the polarization field of the ions ($\hbar\omega_{LO,1} = 0.153\ eV$, $\hbar\omega_{LO,2} = 0.063\ eV$). Electronic Bloch waves can be perturbed by displacement of an ion from its equilibrium position. This causes electrons to interact with the lattice via nonpolar acoustic and optical phonons. The nonpolar optical phonon ($\hbar\omega_{TO} = 0.132\ eV$) is of less importance but allows band-to-band scattering [3],[4]. At low energies electrons can undergo nonpolar acoustic collisions. The scattering rate is approximated by an intraband elastic ansatz [8], whereas at high electron energies U-processes occur stabilizing the electronic transport in SiO_2 [6],[7].

3. The Transport Model

In this section we briefly describe our Monte Carlo algorithm to solve the Boltzmann transport equation (BTE). An excellent review on this method is given in [8]. The equation of motion and the duration of free flight are solved simultaneously by employing a Runge-Kutta algorithm instead of the usual self-scattering scheme. After performing a free flight the scattering process is randomly chosen according to the partial scattering rates. If one scattering process is selected the after-scattering state of the electron is calculated. Having evaluated the state of the scattered electron we perform another free flight till the maximum number of scattering events is reached.

4. Results

To model the band-structure in SiO_2 we implemented an isotropic four-band model with one nonparabolic (nonparabolicity α) and three parabolic bands [9]

$$\epsilon(1+\alpha\epsilon) = \frac{\hbar^2 k^2}{2m^*} \quad \text{for } 0 \le k \le k_{max} \quad \text{band 1,} \tag{1}$$

$$\epsilon = \epsilon_0 \pm \frac{\hbar^2 k^2}{2m^*} \quad \text{for } 0 \le k \le k_{max} \quad \text{band 2,3,4.} \tag{2}$$

band	m^* $[m_e]$	ϵ_1 $[eV]$	ϵ_2 $[eV]$	k_{max} $[nm^{-1}]$	multiplicity
1	0.50	0.00	5.52	11.54	6
2	1.34	5.52	9.31	11.54	6
3	1.05	7.00	9.00	7.42	12
4	1.05	9.00	11.00	7.42	12

Tab. 1: Parameters of the four-band model used

The parameters of our sperical band-structure are summarized in Tab. 1 and were extracted from band calculations of Chelikovsky and Schlüter [10]. The first two conduction-bands were appropriately fitted with respect to an equivalent volume of the first Brillouin zone. Bands three and four crudely account for the behavior of higher conduction-bands due to their parabolic character, but allow a qualitative estimation of their influence on electron transport in oxides.

In Fig. 1 our four-band model is shown. The density of states (Fig. 2) of one parabolic, one nonparabolic and the four-band model are compared, whereas the first bands have the same mass. It is clearly seen for intermediate and high energies that the density of states strongly differs. The main features of a realistic band-structure with two maxima at 5.5 eV and 9 eV and one minimum at 7 eV are well reproduced and strongly influence the electronic distribution at all energies.

Tab. 2 reports the band occupancy of the four-band model. At low electric fields only the first band contributes to electron transport in SiO_2. An occupation of the second band is detected for fields being larger than 2 MV/cm, whereas the third and fourth band are not occupied significantly. The main contribution to the electronic transport behavior in SiO_2 is affected by an appropriate selection of the first conduction-band.

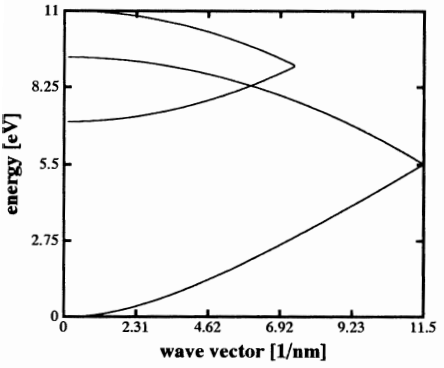

Fig. 1: Band-structure of the four-band model.

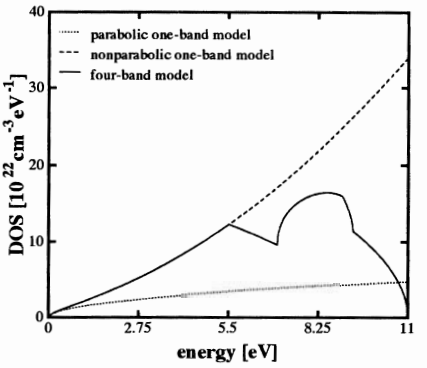

Fig. 2: DOS of the different band-structures.

E [MV/cm]	band 1 [%]	band 2 [%]	band 3 [%]	band 4 [%]
1	100.000	0.000	0.000	0.000
2	100.000	0.000	0.000	0.000
3	99.995	0.005	0.000	0.000
4	99.982	0.108	0.000	0.000
5	99.219	0.780	0.001	0.000
6	97.233	2.759	0.006	0.002
7	92.777	6.200	0.018	0.005
8	89.133	10.810	0.040	0.017
9	84.188	15.716	0.070	0.026
10	79.132	20.717	0.106	0.045

Tab. 2: Band occupancy of the four-band model.

Fig. 3 presents the total scattering rate for a temperature of 300 K and compares it with a single conduction-band. Nonpolar acoustic phonons set in at about 2.75 eV as the dominant scattering process (U-process). Compared with one-band models the different character of the four-band model again results in two maxima and one minimum. The discontinuity at the peak reflects the intravalley character of U-processes.

The dependence of the drift velocity of electronic carriers in SiO_2 versus electric field is plotted in Fig. 4. It increases till U-processes occur. A parabolic one-band model tends to lower velocities, whereas nonparabolicity increases the velocity. The split-off between the nonparabolic band-model and the four-band model is caused by a non-negligible occupancy of the second band at high electric fields. Our data are compared with the results of Fischetti [7]. In Fig. 5 the corresponding mobility in silicon dioxide is presented.

The average energy is plotted in Fig. 6. We observe that a single nonparabolic conduction-band and the four-band model do not exhibit any deviation, moreover, they almost demonstrate quantitative identical values. For data reported in literature [6],[7],[11] three different techniques have been employed to extract the energy as a function of the applied electric field, namely the carrier-separation technique, the electroluminiscence method and finally the vacuum-emission technique. We find a remarkable agreement with experimental data.

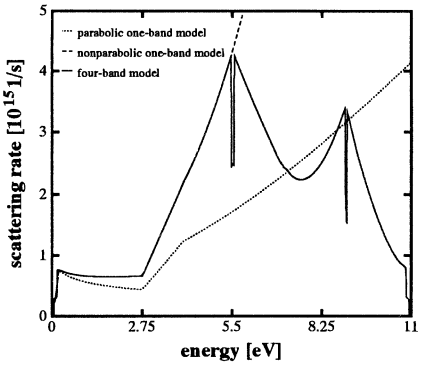

Fig. 3: Scattering rate of SiO_2.

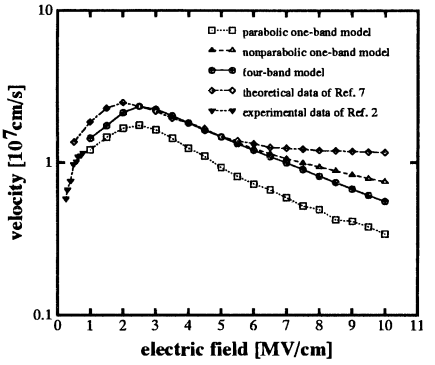

Fig. 4: Drift velocity in SiO_2.

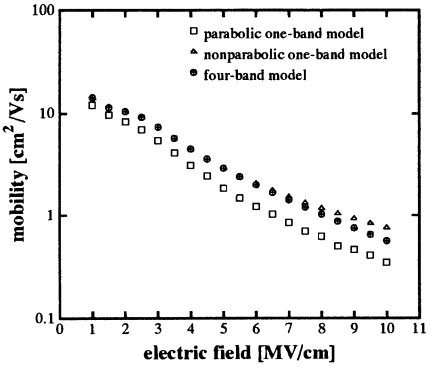

Fig. 5: Mobility in SiO_2.

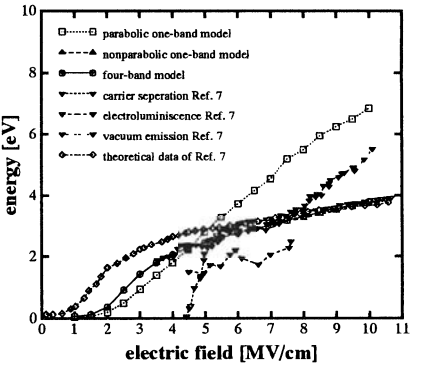

Fig. 6: Average energy in SiO_2.

Acknowledgment

The financial support of SIEMENS Munich, FRG is gratefully acknowledged.

References

[1] W. Porod and D.K. Ferry. *Physical Review Letters*, 54(11):1189–1191, 1985.
[2] H.-J. Fitting and J.-U. Friemann. *Physica status solidi (a)*, 69:349–358, 1985.
[3] H. Köstner Jr. and K. Hübner. *Physica status solidi (b)*, 118:293–301, 1983.
[4] B.K. Ridley. *Journal of Applied Physics*, 46(3):998–1007, 1975.
[5] M. Sparks, D.L. Mills, A.A. Maradudin, L.J. Sham, E. Loh Jr., and D.F. King. *Physical Review B*, 24(6):3519–3536, 1981.
[6] M.V. Fischetti. *Physical Review Letters*, 53(18):1755–1758, 1984.
[7] M.V. Fischetti, D.J. DiMaria, S.D. Brorson, T.N. Theis, and J.R. Kirtley. *Physical Review B*, 31(11):8124–8142, 1985.
[8] C. Jacoboni and L. Reggiani. *Review Modern Physics*, 55(3):645–705, 1983.
[9] R. Brunetti, C. Jacoboni, F. Venturi, E. Sangiorgi, and B. Ricco. *Solid-State Electronics*, 32(12):1663–1667, 1989.
[10] J.R. Chelikowsky and M. Schlüter. *Physical Review B*, 15(8):4020–4029, 1977.
[11] M.V. Fischetti, S.E. Laux, and D.J. DiMaria. *Applied Surface Science*, 39:578–596, 1989.