A Simple Hot Electron Transport Model and its Prediction of Si-SiO_2 Injection Probability

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A simple two band model for hot electron transport in silicon is proposed. The present model can predict correctly not only the drift velocity and impact ionization coefficients of electron as a function of electric field but also the electron Si-SiO_2 injection probability and the quantum yield which have not been properly considered so far in the Monte Carlo simulation.

Two isotropic bands with appropriate E-k relations are introduced such that both the density of state $D(E)$ and the group velocity $U_g(E)$ obtained from the two bands are nearly same with the ones obtained from the full band calculation. Here $U_g(E)$ is the magnitude of the group velocity averaged over the surface of constant energy E, which has been shown to be nearly equal to the average electron group velocity at energy E computed from the full band MC simulation[1]. Considering related symmetric points, two isotropic bands are called 'X(-valley) band' and 'L(-valley) band', respectively. (Band multiplicity for X band(Z_X) and L band(Z_L) are 6 and 8.) The E-k relations for each bands are obtained as follows. Let $E_i(k)$, $D_i(E)$ and $U_{gi}(E)$ be the E-k relation, density of state and magnitude of group velocity with $i = X$ or L, then for an isotropic i-band, we have

$$D_i(E) = \frac{Z_i}{\pi^2}\frac{k^2}{|\frac{dE_i(k)}{dk}|}, \quad U_{gi}(E) = \frac{1}{\hbar}|\frac{dE_i(k)}{dk}| \tag{1}$$

Using Eq. (1), we can show that for each band, k(E) and $U_{gi}(E)$ can be expressed as a function of $D_i(E)$, i.e.,

$$k = (\frac{3\pi^2}{Z_i})^{\frac{1}{3}}(I_i(E))^{\frac{1}{3}}, \quad U_{gi}(E) = \frac{1}{\hbar}(\frac{9Z_i}{\pi^2})^{\frac{1}{3}}\frac{(I_i(E))^{\frac{2}{3}}}{D_i(E)} \tag{2}$$

with $I_i(E) = \int_{E_{i,min}}^{E} D_i(E')a(E')dE'$, where $a(E') = 1$ for the interval of E' with $\frac{dE_i'}{dk} > 0$, and $a(E') = -1$ for the interval of E' with $\frac{dE_i'}{dk} < 0(E_{X,min} = 0eV$ and $E_{L,min} = 1.05eV)$. $E_i(k)$ is determined to satisfy

$$D_X(E) + D_L(E) = D(E), \quad D_X(E)U_{gX}(E) + D_L(E)U_{gL} = D(E)U_g(E) \tag{3}$$

Since $U_{gi}(E)$ can be expressed as a function of $D_i(E)$, using Eq. (3), we can find $D_X(E)$ and $D_L(E)$. Actually $D_X(E)$ and $D_L(E)$ are found by a trial and error method. Then $U_{gi}(E)$ and $E_i(k)$ are subsequently obtained using Eq. (2). $D(E)$ and $U_g(E)$ are calculated using empirical pseudopotential method(EPM) with the band structure parameters in [2]. Figs. 1, 2 and 3 show $D_i(X)$,$U_{gi}(E)$ and $E_i(k)$, respectively. Scattering models and parameters for X band are same as those proposed by Jacoboni et al. for x-valley[3]. Phonon coupling constant and temperature for X-L interband and L-L interband scattering are 4.75 x 10^8(eV/cm) and 525K. Finally all phonon coupling constants(including those for X band) are linearly increased 16% between 2.2 eV and 2.8 eV. Scattering rates are calculated consistently with the proposed E-k relations[4]. Fig. 4 shows the total phonon scattering rate. For impact ionization, the theoretical calculation proposed by Bude et al.[5] is used and second generated carriers are obtained using Kane's random k-approximation with uniformly distributed k-vector[6].

Fig.5 shows the drift velocity and average energy of electron in Si as a function of electric field, where the effect of impact ionization is included. In Fig. 6, we compares the impact ionization coefficients and quantum yield obtained from our model with those of the experimental data[7,8].

Finally, using our two band model, we calculated the electron injection probability from Si into SiO_2 (Ning's experiment[9]), which has not been dealt properly in the MC simulation in spite of its practical significance in the hot carrier reliability modeling. The injection probability of electron is determined by three factors, which include the distribution of electrons approaching Si-SiO_2 interface from bulk, the transmission probability due to thermionic and tunneling emission and the scattering inside SiO_2. For the electron distribution, we simulated the electron trajectory in the substrate electric field profiles given by 2D device simulator for the devices used in the experiment[9]. For the calculation of the transmission probability of electrons from Si into SiO_2, we used the quantum mechanical image-force theory[9] which most correctly explains the internal photoemission and photon-assisted tunneling experiments. The electron transport in SiO_2 was considered using the same transport model used by Fischetti et al.[10], in order to include the back scattering. For the statistical enhancement, the multiplication scheme in real and momentum spaces is used. In Fig. 7, a comparison between measured and calculated injection probabilities for three different devices biased with $F_{ox} = 2MV/cm$ and various substrate voltages is shown. Fig. 8 shows the dependence of injection probability on oxide field. Open circles are the MC results without considering transport in SiO_2 for $V_{sub} = 15V$. As shown in the figures, reasonable agreement for wide range of bias condition is realized.

In this work an isotropic two band silicon model which is simple and useful for high electric field MC simulation is proposed. The transport model is validated by comparing calculations with variety of experimental results including the electron injection probability from Si into SiO_2 in the MOS structures.

References

[1] F. Venturi et al., *IEDM Tech. Dig.*, p.503, 1991.
[2] M.V. Fischetti et al., *IEEE Trans. Elec. Dev.*, vol.38, p.634, 1991.
[3] C. Jacoboni et al., *Rev. Mod. Phys.* Vol.55, p.645, 1983.
[4] T. Vogelsang et al., *J. Appl. Phys.* Vol.70, No.3, p.1494, 1991.
[5] J. Bude, "Monte Carlo Device Simulation: Full Band and Beyond," K. Hess (ed.), Kluwer Academic Publishers, p.27, 1991.
[6] E.O. Kane, Phys. Rev., 159, p.624, 1967.
[7] V. Overstraeten et al., *Solid State Electronics*, Vol.32, p.583, 1970.
[8] C. Chang et al., *J. Appl. Phys.* Vol.57, No.2, p.302, 1985.
[9] T.H. Ning et al., *J. Appl. Phys.* Vol. 48, p.286, 1977.
[10] A. Hartstein et al., *Phys. Rev.* B25, No.12, p.7174, 1982.
[11] M.V. Fischetti et al., *Phys. Rev.* B31, No.12, p.8124, 1985.
[12] C. Canali et al., *Phys. Rev.* B12, p.2265, 1975.

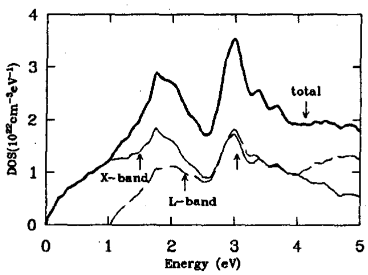

Fig. 1. Total DOS(E) calculated using EPM (thick solid line) is same with the sum of $D_X(E)$ and $D_L(E)$; solid line : $D_X(E)$, broken line : $D_L(E)$.

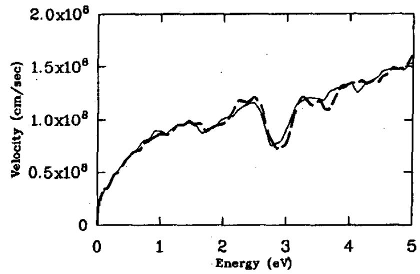

Fig. 2. Electron $U_g(E)$ calculated using EPM (solid line); $U_g(E)$ of present model (broken line).

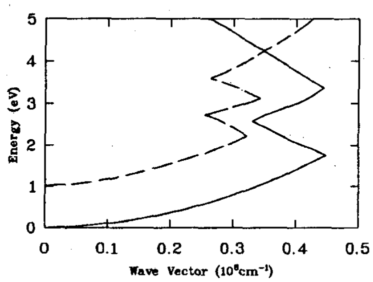

Fig. 3. Generated isotropic E-k relations for X band (solid line) and L band (broken line).

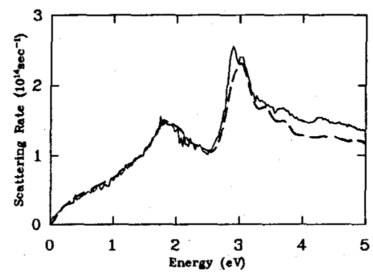

Fig. 4. Total phonon scattering rate : broken line : present model; solid line : Fischetti et al.[2].

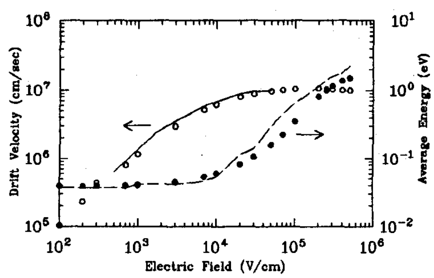

Fig. 5. Electron drift velocity and average energy in bulk silicon computed with the present model (circles); solid line : experimental drift velocity[12], broken line : MC calculated average energy[2].

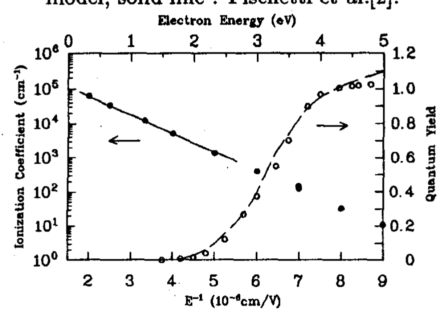

Fig. 6. Impact ionization coefficients and quantum yield; lines : experiments, circles: simulations. Solid line and solid circles : impact ionization[7], broken line and open circles : quantum yield [8]

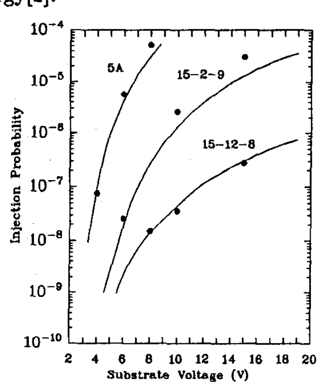

Fig. 7. Injection probability vs. substrate voltage for $E_{ox} = 2MV/cm$ and three different devices. Lines : experiments [8] , circles : simulations.

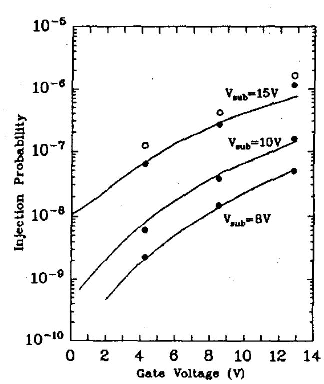

Fig. 8. Injection probability vs. gate voltage for three different substrate voltages. Lines : experiments [9] , circles : simulations.