Verification of Hole Scattering Rates in Si with Quantum Yield Experiment

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High-energy hole scattering rates for a full band Monte Carlo simulation in Si are verified using the quantum yield experiment. We compare two models that yield the correct velocity-field and ionization coefficient characteristics but quite different energy distributions. It is demonstrated that quantum yield experiment is available for a new monitor of hole scattering rates in Si: the model based on *ab initio* impact ionization rate shows good agreements with the experiments.

1. Introduction

High-energy electron scattering models for a full band Monte Carlo (FB-MC) simulation in Si have been extensively studied, and now well recognized scattering rates are determined [1]. On the contrary, much less is known about the hole transport in spite of its importance to the future scaled CMOS technology. This condition is mainly caused by the lack of experimental information about hot hole transport: only two experimental data, *i.e.* drift velocity and ionization coefficient, were available. This study presents a new experimental verification of the hole scattering rates in Si using quantum yield data, which eliminates the uncertainty in determining the scattering rates.

2. Scattering Models

The scattering mechanisms taken account in this study are phonon and impact ionization scatterings, which dominantly characterize the high-field hole transport properties in Si. Figure 1 shows the energy dependent scattering rates for two models compared in this study. Model 1 is based on Jallepalli *et al.*'s work [2], in which both the phonon deformation potentials and the matrix elements for Kane's impact ionization model (random-**k** approximation [3]) are determined by fitting MC calculated drift velocity and ionization coefficient to the experimental results [4, 5]. On the other hand, in Model 2, *ab initio* impact ionization rate reported by Kunikiyo *et al.* [6] are assumed, and only phonon deformation potentials are fitting parameters.

In this study, the following phonon scattering rate has been used:

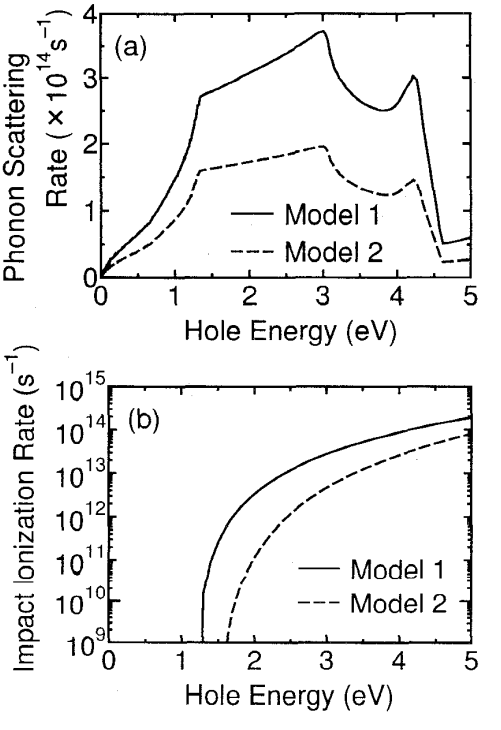

Figure 1: Hole energy dependence of the scattering rates compared in this study. (a) Hole-phonon and (b) hole initiated impact ionization scattering rates.

0-7803-4369-7/98 $10.00

$$\frac{1}{\tau^{\pm}_{\mathrm{ph},\eta}(n,\mathbf{k})} = \sum_{n'}\sum_{\mathbf{q}\in \mathrm{BZ}} \frac{\pi}{\rho\Omega\omega_{\eta,\mathbf{q}}} D_{\eta}(n,\mathbf{k},n',\mathbf{q}) \times \left(N_{\mathbf{q},\eta} + \frac{1}{2} \mp \frac{1}{2}\right) \times \delta(E_{n',\mathbf{k}+\mathbf{q}} - E_{n,\mathbf{k}} \mp \hbar\omega_{\eta},\mathbf{q}), \quad (1)$$

where the upper signs are for absorption and the lower signs are for emission, n and $\mathbf{k}$ are band index and wave vector of the initial hole state, n' is band index of the final hole state, ρ is the crystal density, Ω is the crystal volume, $\omega_{\eta,\mathbf{q}}$ and $N_{\mathbf{q},\eta}$ are the frequency and occupation number of the phonon of branch η with wave vector $\mathbf{q}$, $D_{\eta}(n,\mathbf{k},n',\mathbf{q})$ is the deformation potential, and $E_{n,\mathbf{k}}$ is the hole energy. The dispersion for longitudinal-acoustic (LA), transverse-acoustic (TA) and optical phonons are approximated by the model described in Ref. [8]. The square of deformation potentials are assumed to be linearly dependent on the initial hole energy E as in the FB-MC simulator for electron transport in Si developed by Osaka group [9].

$$D_{\mathrm{TA}}(n,\mathbf{k},n',\mathbf{q}) = D_{\mathrm{LA}}(n,\mathbf{k},n',\mathbf{q}) = (A_{\mathrm{ac}} + B_{\mathrm{ac}}E_{n,\mathbf{k}})^{1/2} \cdot |\mathbf{q}|, \quad (2)$$

$$D_{\mathrm{op}}(n,\mathbf{k},n',\mathbf{q}) = (A_{\mathrm{op}} + B_{\mathrm{op}}E_{n,\mathbf{k}})^{1/2}, \quad (3)$$

where A_{ac}, B_{ac}, A_{op}, and B_{op} are fitting parameters. Values of these parameters for two models are given in Table 1. It should to be noted that in model 1, acoustic phonon scattering has been modeled as an elastic process during the simulation.

Both of two models yield the correct velocity-field and ionization coefficient characteristics as shown in Figs. 2 and 3. However, note that the quite different energy distributions are obtained as shown in Fig. 4, which means that a significant error in the hot hole analysis is caused by the accuracy of scattering rates.

3. Experiments

In order to examine the validity of the scattering rates, we compared experimental quantum yield data larger than unity to the FB-MC simulations. Figure 5 shows the schematic picture of the experimental setup of charge separation technique to measure the quantum yield of impact ionization. The devices used in this study are MOSFETs with n^+-polycrystalline silicon gate fabricated on (100) oriented n-type substrate. The thickness of the gate oxide ranges from 5.8 nm to 16.2 nm and

Table 1: Numerical values of parameters for the phonon deformation potentials.

Parameters	Model 1	Model 2	Units
A_{ac}	5.28	4.0	eV^2
B_{ac}	0	-0.35	eV
A_{op}	2.5×10^{17}	1.0×10^{17}	$\mathrm{eV}^2\mathrm{cm}^{-2}$
B_{op}	0	5.0×10^{15}	eVcm^{-2}

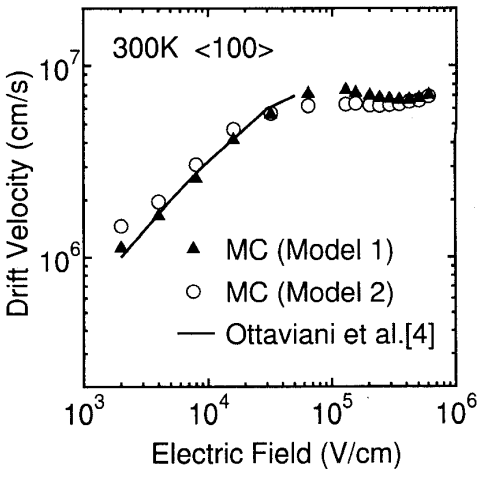

Figure 2: Experimental and simulated hole drift velocity at room temperature as a function of electric field along the ⟨100⟩ crystallographic direction.

channel doping density is 2×10^{17} cm^{-3}. Quantum yield, γ, is defined as the number of electron-hole pairs generated by a hot electron [7]. As shown in Fig. 6, electrons are injected from the gate into the oxide layer by Fowler-Nordheim tunneling. As they enter the Si substrate after traveling in SiO_2, they generate electron-hole pairs. The number of pairs can be derived from the ratio of the channel (hole) current to the gate (electron) current. The experimental data of γ as a function of oxide voltage are shown in Fig. 7. In thinner oxides ($t_{\mathrm{ox}} \leq 7.4$nm), universal relationship between γ and the oxide voltage are found irrespective of the oxide thickness [10]. This indicates ballistic transport of electrons inside SiO_2, and we

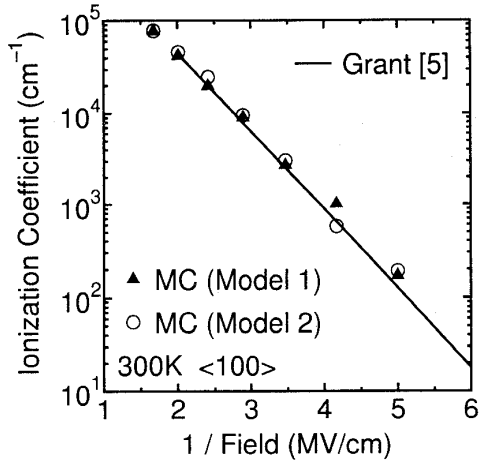

Figure 3: Experimental and simulated impact ionization coefficient at room temperature for a field along the ⟨100⟩ crystallographic direction.

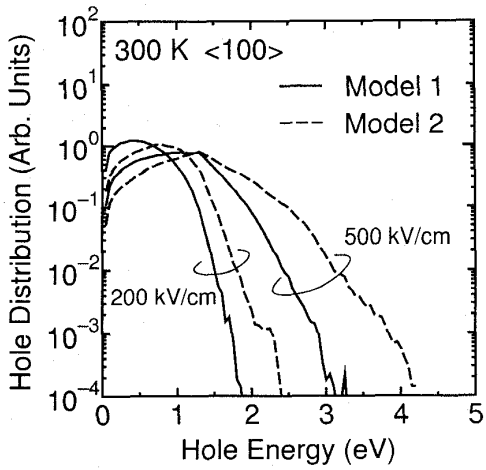

Figure 4: Calculated hole energy distributions at room temperature in the homogeneous electric fields along the ⟨100⟩ crystallographic direction.

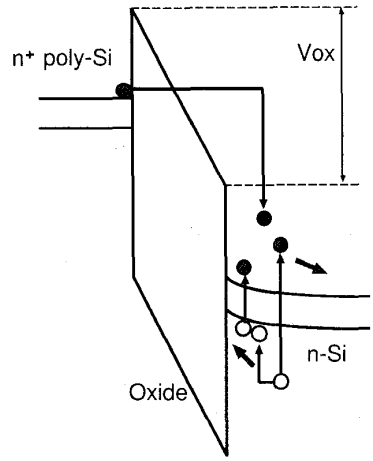

Figure 6: Schematic energy band diagram illustrating quantum yield experiment. This figure shows two impact-ionization events initiated by an electron injected from SiO_2 and a secondary generated hole.

can hence easily obtain the energy of electrons injected into Si without any knowledge of electron transport in SiO_2.

4. Simulation of Quantum Yield

The FB-MC simulation for both electron and hole relaxation processes in Si using Kunikiyo *et al.*'s electron transport model [9] and two hole transport models described in Sec. 2 has been performed. The effect of the electric field in the surface depletion region is taken account [11] because the substrate doping concentration is relatively high. Simulated results are shown in Fig. 7 with lines. Lower γ obtained from the simulation without the hole initiated impact ionization process indicates that secondary generated holes can produce additional pairs if they have enough energy. The calculated results with hole transport model 2 show good agreement with experiments, whereas those with model 1 do not. This supports the theoretical idea that random-**k** approximation overestimates the impact ionization rate near threshold [12], which significantly promotes the pair production events initiated by secondary holes.

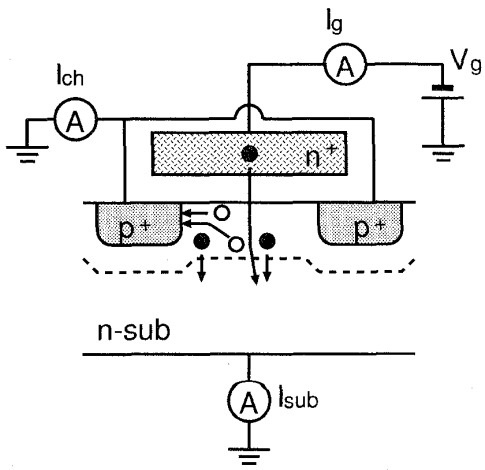

Figure 5: Schematic picture of the experimental setup of charge separation technique to measure the quantum yield of impact ionization. Closed and open circles represent electrons and holes, respectively.

5. Conclusion

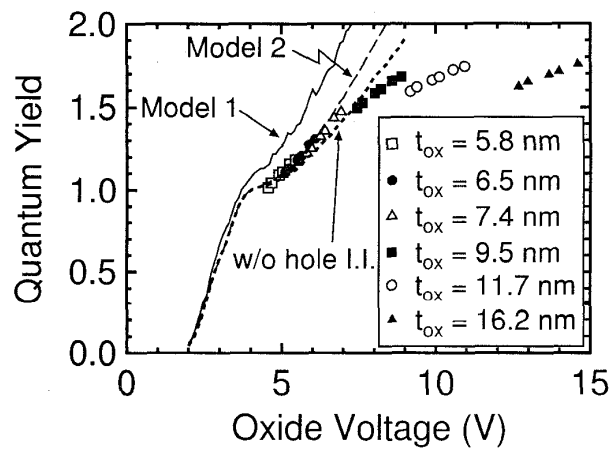

Figure 7: Experimental (symbols) and calculated (lines) data of quantum yield as a function of oxide voltage.

In summary, we have demonstrated that quantum yield experiment is available for the monitor of hole scattering rates in Si. The model based on *ab initio* impact ionization rate shows fairly good agreements with the experiments.

Acknowledgements

One of the authors (Y.K) gratefully acknowledge T. Iizuka and Y. Yamamoto of NEC Corporation for many valuable comments and discussions on the hot carrier transport in Si.

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