Analysis of Hot-Carrier-Induced Oxide Degradation in MOSFETs by Means of Full-Band Monte Carlo Simulation

Yoshinari Kamakura, Kazuaki Deguchi, and Kenji Taniguchi
Department of Electronics and Information Systems, Osaka University
2-1 Yamada-oka, Suita, Osaka 565-0871, Japan
E-mail: kamakura@eie.eng.osaka-u.ac.jp

Abstract

We demonstrate the investigations of oxide reliability by means of full-band Monte Carlo simulation. Firstly we discuss the accuracy of the scattering rates particularly for hot hole transport. It is shown that the quantum-yield experiment provides a means to verify the scattering models for hot carriers in MOS system. Secondly, the oxide breakdown is studied by using a substrate hot electron injection technique. Monte Carlo simulations are performed to examine the correlation between the oxide breakdown and the electron energy, and it is shown that the holes generated in the anode electrode play an important role in the oxide degradation. In addition, it is discussed that rigorous hot carrier simulations are necessary to study the reliability issues for ultra-thin oxide films used in advanced CMOS technology.

1 Introduction

The reliability of gate oxide is a major concern for further downscaling of MOS devices (Degraeve et al. 2000). Understanding the mechanism of oxide degradation and final breakdown is essential for accurate projection of oxide reliability. Many previous works (Chen et al. 1986, DiMaria et al. 2001) have pointed out that the hot carriers injected into the gate oxide originate the oxide degradation. Thus the rigorous modeling of the hot carrier behavior in MOS system is very important, e.g., to confirm the validity of the empirical projection manner using accelerated lifetime tests. In order to simulate the hot carrier transport in semiconductors using fewer assumptions and approximations, a full-band Monte Carlo (FBMC) technique has been extensively studied since the early 1980s (Shichijyo and Hess 1981, Fischetti and Laux 1988). Recently, the state-of-the-art FBMC simulators have been utilized by several groups for analyzing the oxide degradation (Bude et al. 1998, Ezaki et al. 2000). In the present work, we will firstly discuss the accuracy of the scattering models particularly for hot hole transport, which plays a key role in the oxide degradation. Then we demonstrate an example for the application of FBMC to studying oxide reliability, i.e., the investigation of breakdown induced by substrate hot electron (SHE) injection.

2 Verification of scattering models for FBMC simulation

In this work, we solve the Boltzmann transport equation for both electrons and holes in Si using a FBMC technique (Kunikiyo et al. 1994). The realistic band structure and the scattering rates essential for the hot carrier analysis, i.e., phonon scattering and impact ionization, are taken into account. All scattering rates have been derived on the basis of the band calculation (Cohen and Bergstresser 1966) and the resulting density of states. Figure 1 shows the scattering rates employed in our simulator. We used the electron scattering models reported by Kunikiyo et al. (1994), which are almost the same as those employed in the FBMC simulators of other groups (Abramo et al. 1994). They have been verified with various experimental data, e.g. the drift velocity, the ionization coefficient and the quantum yield, the soft x-ray photoemission spectroscopy, etc. (Cartier et al. 1993). On the other hand, although it has been pointed out that the hole holes significantly affects the oxide reliability, much less is known about the hole transport in Si (Kamakura et al. 2000). We assumed the theoretically computed ionization rate reported by Kunikiyo et al. (1996), and the phonon deformation potentials are determined by fitting the simulated drift velocity and the ionization coefficient to the experimental results (Ottaviani et al. 1975, Grant 1973). The states of secondary carriers after the impact ionization are obtained from the random-k approximation (Kane 1967).

In order to verify the scattering models, particularly for the hot hole transport, we simulated the quantum yield of the impact ionization. Quantum yield γ is defined as the number of electron-hole pairs generated by an injected hot electron (Chang et al. 1985). γ gives information about the ratio between the ionization and the phonon scattering rates, and hence it has played an important role in determining the scattering rates for hot electrons in Si (Cartier et al. 1993). γ as a function of electron energy can be measured by the charge separation technique as shown in Fig. 2. The number of pairs is derived from the ratio

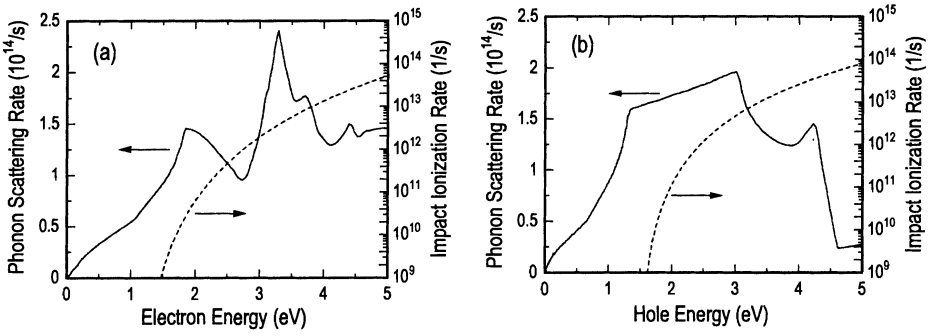

Fig. 1. (a) Scattering rates for (a) electrons and (b) holes in Si at room temperature. Total phonon scattering rate (solid line) and impact ionization rate (dashed line) are plotted as a function of carrier energy.

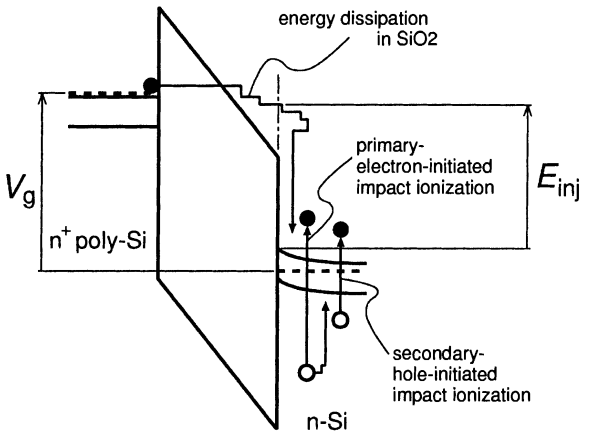

Fig. 2. Schematic energy band diagram illustrating quantum-yield experiment in FN tunneling regime.

of the channel (hole) current to the gate (electron) current of p-MOSFET. In this study our attention was focused on γ exceeding unity, which is obtained in the Fowler-Nordheim (FN) tunneling regime. Due to the high oxide voltage (> 3.2 V), the electrons are injected into the Si with high kinetic energies, and the secondary generated particles after impact ionizations can gain sufficient energy to produce additional pairs. The resulting γ contains the desired information about the impact ionization events induced by the secondary holes. We performed quantum-yield experiments by using MOSFETs with a heavily doped ($\simeq 8 \times 10^{17}$ cm^{-3}) Si substrate. Figure 3 (a) shows the experimental

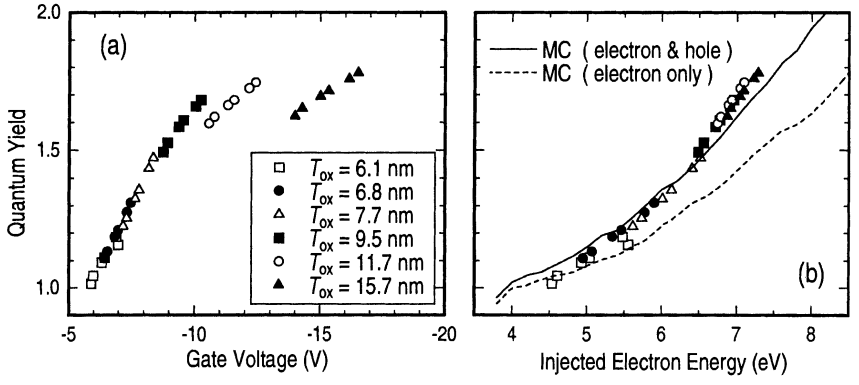

Fig. 3. (a) Measured γ as a function of gate voltage for the samples having various oxide thicknesses. (b) γ as a function of E_{inj}. Simulated results taking account of electron-initiated ionization process only (dashed line) and both electron- and hole-initiated ionization processes (solid line) are compared.

γ for various oxide thicknesses ranging from 6.1 to 15.7 nm. In thinner oxides ($t_{ox} \leq 7.7$ nm), a universal relationship between γ and V_g is found, irrespective of the oxide thickness indicating quasiballistic transport inside SiO_2. On the other hand, $\gamma - V_g$ characteristics for thicker oxides depend on thickness because of the strong energy dissipation in SiO_2. In the present study, we computed the initial electron energy immediately after the injection into Si, E_{inj}, by performing MC simulations in SiO_2 (Arnold et al. 1994). Note that a universal relationship irrespective of the oxide thickness is obtained, which ensures the validity of E_{inj} evaluation. The simulated results taking account of both electron- and hole-initiated impact ionization processes show good agreements with experiments. In this way, the quantum-yield experiment provides a means to verify the scattering models for not only hot electrons in Si but also hot holes in Si and hot electrons in SiO_2, whose accuracy significantly affects the modeling of oxide degradation.

3 Analysis of oxide reliability using FBMC simulations

3.1 Oxide breakdown induced by SHE injection

FN tunneling injection has been widely used to study the time-dependent dielectric breakdown of gate oxide films. During the FN stress as shown in Fig. 4 (a), hole current is observed at the substrate electrode. It has been suggested that this is caused by the hot hole injection from the anode interface. Experiments have shown that an oxide's lifetime t_{BD} can be projected from the time required for the hole fluence to reach some critical value Q_p, independent of the gate voltage (Chen et al. 1986):

$$\int_0^{t_{BD}} J_p(t)\, dt \equiv Q_p, \tag{1}$$

where $J_p(t)$ is the substrate hole current divided by gate area. This observation is the experimental basis for the anode-hole injection model, in which the oxide breakdown is explained by considering that holes are responsible for the damage

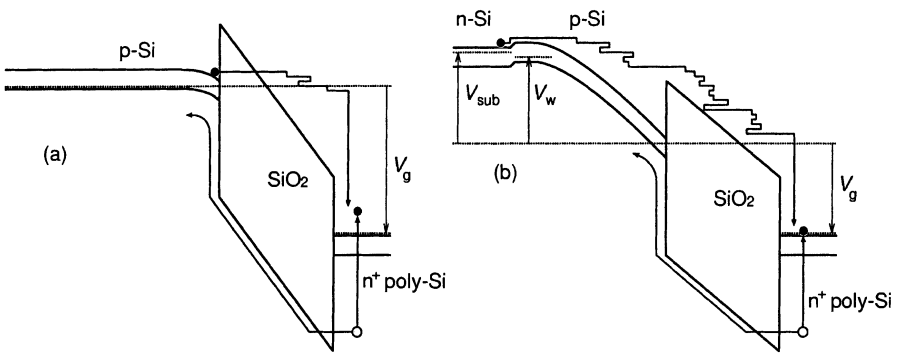

Fig. 4. Schematic energy band diagram illustrating (a) FN and (b) SHE injection.

leading to oxide degradation and final breakdown (Degraeve et al. 1998). However, because FN injection needs high oxide field (> 10 MV/cm), it is possible to consider that the electric field itself causes the damage creation (McPherson et al. 2000). In this study we investigated oxide breakdown using a different stress technique, i.e., SHE injection, with which we can independently control the oxide field and carrier energy. Figure 2 (b) shows the schematic energy band diagram illustrating SHE injection. Cold electrons, injected into the p-Si layer from the n-Si by forwardly biasing, are accelerated towards the Si/SiO_2 interface, and some of them gain sufficient energy to surmount the Si/SiO_2 barrier. Because the hole current through the oxide layer cannot be separated from the electron current, it is impossible to verify experimentally whether the holes also control the oxide breakdown induced by SHE stress. We calculated the hole current theoretically by means of MC simulation, and investigated the origin of the oxide degradation that eventually triggers the destructive breakdown.

The devices used are n-MOSFETs having conventional SiO_2 gate oxide, n^+ poly-Si gates, p-Si wells, and n-Si substrates. The oxide thickness is 5 nm, and the channel doping concentration is $5 \times 10^{17}cm^{-3}$. By using FN and SHE injection, we measured the gate current as a function of stress time until the occurrence of the oxide breakdown. In order to evaluate the hole current through the oxide layer, FBMC simulations were performed for the electron heating in the Si substrate and energy relaxation processes of electrons and holes in the poly-Si gate. Electrons in SiO_2 are computed with an analytical band MC model reported by Arnold et al. (1994). The hole injection into SiO_2/poly-Si barrier, which is lowered by an image force effect, is calculated with the tunneling probability based on the WKB approximation. Figure 5 shows the experimental charge-to-breakdown Q_{BD} as a function of V_g for FN and SHE injections. Q_{BD} is defined as the total charge fluence through the oxide layer until the occurrence

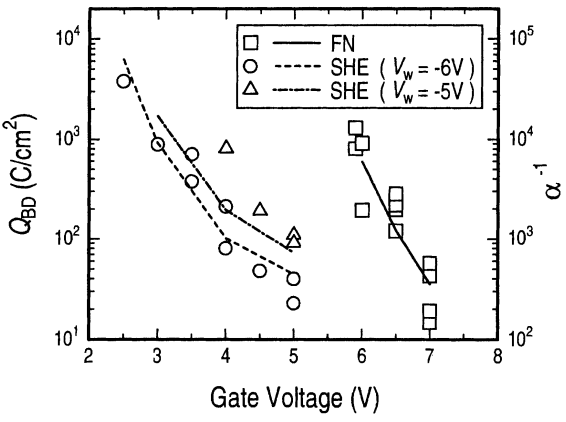

Fig. 5. Experimental Q_{BD} (symbols) and calculated α^{-1} (lines) as a function of gate voltage.

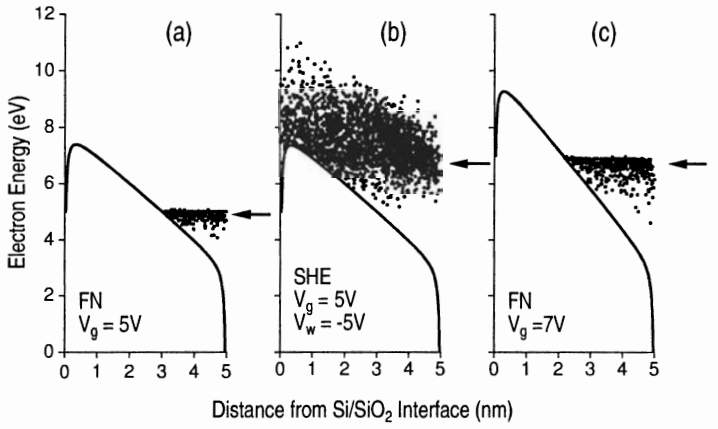

Fig. 6. Snapshots of the simulated electrons in the oxide layer for various stress conditions. The heavy lines indicate the conduction band edge of the gate oxide, and the energy is measured from the bottom of the conduction band in the gate poly-Si.

of the breakdown. The dependence of Q_{BD} on the bias conditions and the injection techniques can be understood in terms of the electron energy. Figure 6 shows the snapshots of the simulated electrons in the oxide layer. Under the same V_g (= 5 V) the electron energy at the anode interface for FN injection is much higher than that of SHE injection as shown in Figs. 6 (a) and 6 (b). In Fig. 5, Q_{BD} for FN injection is also much larger than that of SHE injection. We have to apply higher V_g for FN injection (see Fig. 6 (c)) to obtain the energy distribution similar to SHE injection. Note that under these conditions Q_{BD} for both injection techniques are comparable. These results indicate the strong correlation between the oxide breakdown and the electron energy at the anode. For further examination to the degradation mechanism, we computed the hole injection from the anode interface. In Fig. 5 we plot the simulated results of the inverse of the hole injection efficiency $J_p/J_g \equiv \alpha$, where J_g is the gate current density. On the basis of the anode-hole injection model, Q_{BD} is related to Q_p as $Q_{\mathrm{BD}} = Q_p/\alpha$. Good agreement between experiment and simulation is obtained with the same Q_p regardless of the injection technique. This indicates that the anode hole injection also controls the oxide's lifetime stressed by SHE injection.

3.2 Reliability projection of ultra-thin oxide

The aggressive scaling of oxide thickness into direct-tunneling regime has drastically reduced the margin for error in reliability projection (Degraeve et al. 2000). In order to understand how to extrapolate the results of accelerated lifetime tests to operation voltage, the mechanism of oxide degradation must be understood exactly. Even if we assume the anode-hole injection model, the situation is not so easy as for thicker oxides. Recent experiments have demonstrated that a strong

correlation exists between the degradation of ultra-thin oxides and the hole energy injected by direct tunneling (Deguchi et al. 2000). That is, the lifetime of ultra-thin oxide (< 3 nm) is a function of not only the hole fluence as assumed in Sec. 3.1, but also the hole energy. Moreover, this means that the channel hot holes can create oxide defects via direct tunneling even though they have insufficient energy to surmount the energy barrier (DiMaria et al. 2001). The rigorous modeling of hot carrier behavior in Si is still important for discussing the reliability issues of advanced CMOS technology using reduced supply voltage.

4 Conclusion

We have demonstrated that the FBMC simulation is a very helpful tool for investigating the mechanism of oxide degradation. The MC simulator, whose accuracy have been verified by the quantum-yield experiment, has been utilized to analyze the oxide breakdown induced by FN and SHE injections. The strong correlation between the oxide breakdown and the electron energy was found, and it was shown that the holes generated in the anode electrode play an important role in the oxide degradation. In addition, it was indicated that the rigorous modeling of hot carrier behavior in Si is still important for discussing the reliability of aggressively scaled oxide films used in advanced CMOS technology.

Acknowledgement

This work was supported by Semiconductor Technology Academic Research Center (STARC).

References

[1] Abramo, A. , Baudry, L., Brunetti, R., Castagne, R., Charef, M., Dessenne, F., Dollfus, P., Dutton, R., Engl, W.L., Fauquembergue, R., Fiegna, C., Fischetti, M.V., Galdin, S., Goldsman, N., Hackel, M., Hamaguchi, C., Hess, K., Hennacy, K., Hesto, P., Higman, J.M., Iizuka, T., Jungemann, C., Kamakura, Y., Kosina, H., Kunikiyo, T., Laux, S.E., Lin, H., Maziar, C., Mizuno, H., Peifer, H.J., Ramaswamy, S., Sano, N., Scrobohaci, P.G., Selberherr, S., Takenaka, M., Tang, T.-W, Taniguchi, K., Thobel, J.L., Thoma, R., Tomizawa, K., Tomizawa, M., Vogelsang, T., Wang, S.-L., Wang, X., Yao, C.-S., Yoder, P.D., Yoshii, A. (1994): A comparison of numerical solutions of the Boltzmann transport equation for high-energy electron transport silicon. IEEE Trans. Electron Devices 41: 1646-1654

[2] Arnold, D., Cartier, E., DiMaria, D.J. (1994): Theory of high-field electron transport and impact ionization in silicon dioxide. Phys. Rev. B 49: 10278-10297

[3] Bude, J.D., Weir, B.E., Silverman, P.J. (1998): Explanation of stress-induced damage in thin oxides. In: Technical Digest of International Electron Devices Meeting, IEDM '98, San Francisco, CA. IEEE, Piscataway, pp. 179-182

[4] Cartier, E., Fischetti, M.V., Eklund, E.A., McFeely, F.R. (1993): Impact ionization in silicon. Appl. Phys. Lett. 62: 3339-3341

[5] Chang, C., Hu, C., Brodersen, R.W. (1985): Quantum yield of electron impact ionization in silicon. J. Appl. Phys. 57: 302-309

[6] Chen, I.C., Holland, S., Young, K.K., Chang, C., Hu, C. (1986): Substrate hole current and oxide breakdown. Appl. Phys. Lett. 49: 669-671

[7] Cohen, M.L., Bergstresser, T.K. (1966): Band structures and pseudopotential form factors for fourteen semiconductors of the diamond and zinc-blende structures. Phys. Rev. 141: 789-796

[8] Degraeve, R., Groeseneken, G., Bellens, R., Ogier, J.L., Depas, M., Roussel, P.J., Maes, H.E. (1998): New insights in the relation between electron trap generation and the statistical properties of oxide breakdown. IEEE Trans. Electron Devices 45: 904-911

[9] Degraeve, R. (ed.) (2000): Topical issue on oxide reliability. Semicond. Sci. Technol. 15: 425-490

[10] Deguchi, K., Ishida, A., Uno, S., Kamakura, Y., Taniguchi, K. (2000): Degradation of direct-tunneling gate oxide under hot-hole injection. Appl. Phys. Lett. 77: 1384-1386

[11] DiMaria, D.J., Stathis, J.H. (2001): Anode hole injection, defect generation, and breakdown in ultrathin silicon dioxide films. J. Appl. Phys. 89: 5015-5024

[12] Ezaki, T., Nakasato, H., Yamamoto, T., Hane, M. (2000): Simulation of hot hole currents in ultra-thin silicon dioxides: the relationship between time to breakdown and hot hole currents. In: Proceedings of the 2000 International Conference on Simulation of Semiconductor Processes and Devices, SISPAD 2000, Seattle, WA. IEEE, Piscataway, pp. 34-37

[13] Fischetti, M.V., Laux, S.E. (1988): Monte Carlo analysis of electron transport in small semiconductor devices including band-structure and space-charge effects. Phys. Rev. B 38: 9721-9745

[14] Grant, W.N. (1973): Electron and hole ionization rates in epitaxial silicon at high electric fields. Solid-State Electron. 16: 1189-1203

[15] Kamakura, Y., Kawashima, I., Deguchi, K., Taniguchi, K. (2000): Verification of hot hole scattering rates in silicon by quantum-yield experiment J. Appl. Phys. 88: 5802-5809

[16] Kane, E.O. (1967): Electron scattering by pair production in silicon. Phys. Rev. 159: 624-631

[17] Kunikiyo, T., Takenaka, M., Kamakura, Y., Yamaji, M., Mizuno, H., Morifuji, M., Taniguchi, K., Hamaguchi, C. (1994): A Monte Carlo simulation of anisotropic electron transport in silicon including full band structure and anisotropic impact-ionization model. J. Appl. Phys. 75: 297-312

[18] Kunikiyo, T., Takenaka, M., Morifuji, M., Taniguchi, K., Hamaguchi, C. (1996): A model of impact ionization due to the primary hole in silicon for a full band Monte Carlo simulation. J. Appl. Phys. 79: 7718-7725

[19] McPherson, J.W., Khamankar, R.B., A.Shanware, A. (2000): Complementary model for intrinsic time-dependent dielectric breakdown. J. Appl. Phys. 88: 5351-5359

[20] Ottaviani, G., Reggiani, L., Canali, C., Nava, F., Quaranta, A.A. (1975): Hole drift velocity in silicon Phys. Rev. B 12: 3318-3329

[21] Shichijo, H., Hess, K. (1981): Band-structure-dependent transport and impact ionization in GaAs, Phys. Rev. B 23: 4197-4207