Statistical Monte Carlo Simulation for Dielectric Breakdown of Oxide Thin films: Effect of Non-Uniformity of Electron Trap Getenration

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

Abstract This paper introduces a new simulator to investigate the statistical characteristics of dielectric breakdown of silicon dioxide thin films in MOSFETs. Breakdown phenomena are well simulated using the percolation concept. Simulations are carried out taking account of various effects which are physically probable, and statistical properties of simulated breakdown phenomena are studied applying Weibull statistics. A new plotting method is also proposed which is very useful to know what physical effects are accelerated by specific process conditions. Finally, we evaluate the effects of oxynitridation process on dielectric breakdown mechanisms.

1 Introduction

For higher reliability of gate oxide layers in aggressively scaled MOSFETs, it is now strongly required to understand the mechanisms of the dielectric breakdown of gate thin films. Degraeve et al.[1] proposed a model to predict the statistical characteristics of breakdown events using a percolation concept, and they successfully reproduced the experimental cumulative failure (Weibull) curves of conventional oxide films. In their work, they assume uniform generation of electron traps, and hence the constant critical electron trap density (CETD) independent on the stress voltage [1]. However, it has been pointed out that CETD strongly depends on the stress voltage by the study utilizing the A-mode stress induced leakage current (A-mode SILC) [2]. We consider non-uniform distributions such as depth profile [2, 3, 4] and enhanced trap generation around existing traps [5] as the main reason for the stress voltage dependence of CETD. In this work, we systematically investigated the impacts of trap radius as well as these effects on the statistics of breakdown phenomena. A new powerful plotting method is also introduced which can clearly visualize the cause of the change in the Weibull distributions for various oxide thin films.

2 Percolation Model

Dielectric breakdown of silicon dioxide thin films can be simulated using the percolation concept. It is schematically illustrated in Fig. 1. In this model, oxide layer is replaced by three-dimensional space, and spherical electron traps of effective radius r are randomly generated in this volume. With increasing traps, conductive path is produced from the top of the oxide layer to the bottom. This is called "percolation" because electrons can percolate through the oxide layer along this conductive path. Then breakdown phenomena corresponds to percolation in the context of this model. In order to examine the breakdown statistics, three kinds of percolation models are presented in this study.

2.1 Uniform Model

In Degraeve's original work, electron traps are assumed to be generated uniformly in the films. This means that the trap generation probability function p is constant in space:

$$p = \text{constant}. \tag{1}$$

Effective radius r of electron traps is an important factor in this model. Uniform model with $r = 0.45$ nm successfully explains oxide thickness dependence of statistical characteristics for conventional silicon dioxide layer. However it cannot explain the statistics for other films fabricated in different process conditions. The effective radius is subject to many physical aspects of an oxide film and can vary with oxidation conditions, and we should take the effect of different r into account.

2.2 Exponential Model

In exponential model, traps are generated exponentially decaying from Si/SiO_2 interface [3]. In this case, trap generation probability functions are in the form:

$$p = Ne^{-CZ}, \tag{2}$$

where Z is the distance from Si/SiO_2 interface, N is normalization factor, and C represents the decay of trap density from the interface.

2.3 Localization Effect Model

In localization effect model, traps are more likely generated near the other traps. We define p as a function of the distance from other existing traps:

$$p = \begin{cases} E \times N & \text{(Within } 2r \text{ from existing traps)} \\ N & \text{(Other case)}, \end{cases} \tag{3}$$

where E is set lager than unity because existing traps enhance trap generation near them. N is determined by normalization integral. We can simulate how existing traps affect the next trap generation with this parameter E.

Introduction of these three effects results in the different trap distributions at the breakdown as shown in Fig 2. In order to study them, we use some statistical methods which are very useful for the study of dielectric breakdown in oxide films.

3 Weibull Distributions

Statistical properties of breakdown phenomena are well discribed by Weibull distributions. The probability density functions $f(t)$ and cumulative failure functions $F(t)$ of statistical variable t are written in the form

$$f(t) = \frac{\beta}{\theta}\left(\frac{t}{\theta}\right)^{\beta-1} \exp\left[-\left(\frac{t}{\theta}\right)^{\beta}\right], \tag{4}$$

$$F(t) = \int_0^t f(t)dt = 1 - \exp\left[-\left(\frac{t}{\theta}\right)^{\beta}\right], \tag{5}$$

where β and θ are called "*shape parameter*" and "*scale parameter*" respectively. Any Weibull distribution is quantitatively specified by the set of these two parameters. One of Weibull distributions ($\beta = 10$, $\theta = 100$) is shown in Fig. 3 (a). The probability density function of Gaussian distribution having the same mean value and standard deviation is plotted for comparison. It is important to note that two Weibull parameters can be clearly evaluated. From Eq. (5), We obtain

$$W \equiv \ln[-\ln[1 - F(t)]] = \beta[\ln t - \ln \theta]. \tag{6}$$

When we plot Weibull distributions on $W - \ln t$ plane, data lie on straight lines as shown in Fig. 3 (b). This plotting method is useful in analyzing statistical properties of Weibull distributions, and called "*Weibull Plots*". The slope of the straight line is equivalent to Weibull scaling parameter β and the cross section between the straight line and horizontal axis is θ.

4 Simulation Result

4.1 Statistical Properties of Simulated Breakdown Phenomena

A simulator was developed on the basis of the percolation concept. It simulates threshold voltage shifts ΔV_{th}, which gives the experimental information about generated trap profiles for given parameters R, E, and C. We also calculated cumulative failure rate by repeating breakdown simulation for 200 times. Oxide thickness was set 8.9 nm and gate area 900 nm^2. In Fig. 4 we compared the Weibull plots of breakdown distributions simulated with three effects with effective radius r of 0.45 nm. The differences for the three models are clearly observed. In order to clarify the differences of Weibull distributions caused by three effects, it is most appropriate to trace the changes of two Weibull parameters β and θ. Figure 5 is $\theta - \beta$ plot which shows simulated changes for the same films as in Fig. 4. The changes of distributions caused by three effects are more easily understood in this figure. Futhermore, three effects are independent on each other. It is shown in Fig. 6 for the effects of C and E. Solid lines represent the changes induced by local enhancement and dashed lines show the changes by exponential decay of trap profile. The isolation and independence of three effects suggest a new evaluation method by which we can analyze the main physical reason for the changes in Weibull distributions.

4.2 Analysis Method and Application

As is noted in Sec. 4.1, the plotting method shown in Fig. 5 is very powerful to visualize the changes and the differences of Weibull distributions. By plotting breakdown distributions for different process conditions in this way, we can distinguish which effect is most strongly accelerated by each process, and this can be very valuable information on breakdown phenomena. Before applying this plotting method to the analysis of measured data, it is very important to note that θ is dependent on the gate area [6]. The ratio of parameter θ_1 to θ_2 for two samples with different areas A_1, A_2 is written in the form:

$$\frac{\theta_1}{\theta_2} = \left(\frac{A_2}{A_1}\right)^{1/\beta}, \tag{7}$$

so that the simulated data and measured data should be of the films having the same gate area. Figure 7 shows the simulation result for 7 nm-thick oxide films and experimental data from Ref. [7]. Data is taken for silicon oxynitrided films fabricated with different amount of nitridation. Sample 1 is a conventional dioxide film without oxynitridation, but samples 2 - 4 were annealed in a little nitride atmosphere. And sample 5 is a heavily oxynitrided film. From this plot, oxynitridation process can be related with localization effect; it can enhance trap generation near the existing traps. And annealing process can be associated with exponential trap profile effect; it can enhance the trap creation near Si/SiO_2 interface. Of course other effects might be considered as well as three effects examined in this paper, and this method will still give a helpful insight into breakdown phenomena.

5 Conclusion

The impact of three effects (exponential profile, localization effect of electron traps, and the change in the effective radius) has been systematically investigated using a newly developed percolation model. A new plotting method has also been proposed which allows the simple and powerful analysis of the change in Weibull distributions caused by various physical effects. This method will surely give us a breakthrough in the study of dielectric breakdown in oxide thin films.

6 Acknowledgment

The authors are indebted to STARC for their support.

References

[1] R. Degraeve *et al.*, IEDM Tech. Dig., pp.863-866, 1995.

[2] K. Okada *et al.*, Symp. on VLSI Tchnol. Tech. Dig. pp.158-159, 1998.

[3] Q. D. Khosru *et al.*, Conf. SSDM(1991) pp. 14-16.

[4] J. H. Stathis, Microelectronic Engineering, vol.36, pp.325-328, 1997.

[5] T. Tanamoto *et al.*, Jpn. J. Appl. Phys., pp.1439-1442, 1997.

[6] D. R. Wolters and J. F. Verwey, "Breakdown and wear-out phenomena in SiO_2 films," in *Instabilities in Silicon Devices*. Amsterdam, The Netherlands: Elsevier, 1986, ch. 6.

[7] R. Degraeve *et al.*, IEDM Tech. Dig., pp.327-330, 1996.

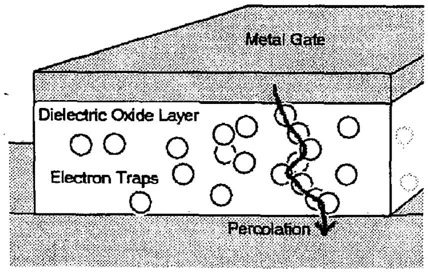

Fig. 1 Schematic illustration of the percolation model for dielectric breakdown of gate oxides in Si-MOSFETs.

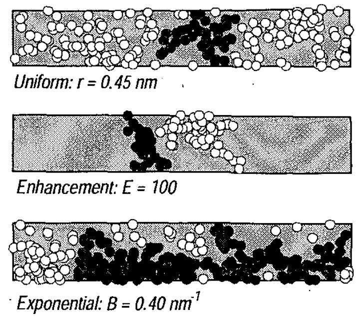

Fig. 2 Simulated distributions of traps at breakdown for three models. Shaded cluster indicates a percolation path.

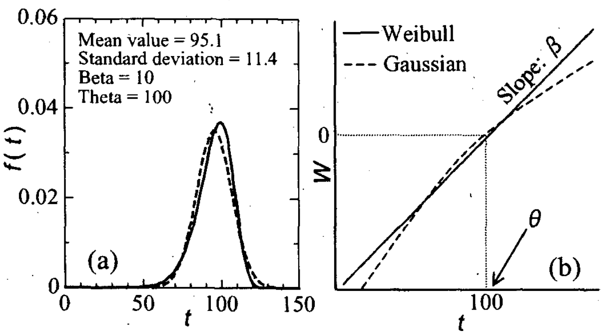

Fig. 3 (a) Weibull distribution for $\beta=10$ and $\theta=100$ (solid line) and corresponding Gaussian distribution (dashed line). Weibull distribution is not symmetrical in contrast to Gaussian distribution. (b) Comparison of two distributions on Weibull plots.

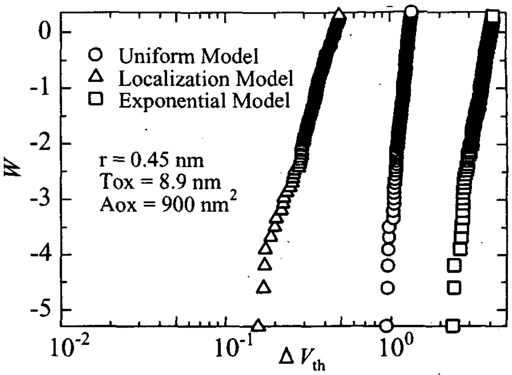

Fig. 4 Weibull plots of critical threshold voltage shifts simulated with three models given in Fig. 2. Both of two parameters for Weibull plots, i.e. θ and β, are different among three models.

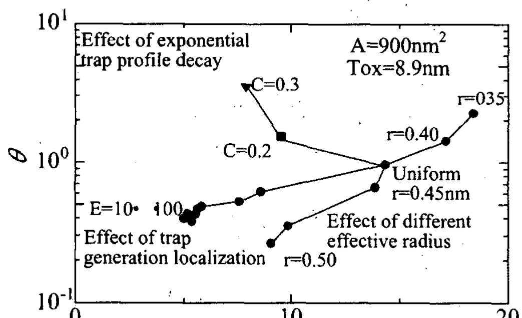

Fig. 5 The θ - β plots of the Weibull distributions simulated with one of the three effects employed in this study.

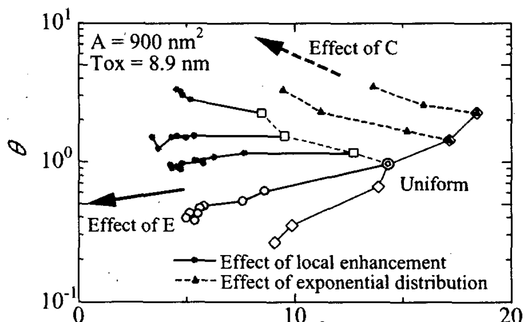

Fig. 6 The θ - β plots of the Weibull distributions by taking account of two effects simultaneously (closed symbols). Note that the directions of the variations induced by one effect are determined regardless of the inclusion of another effect.

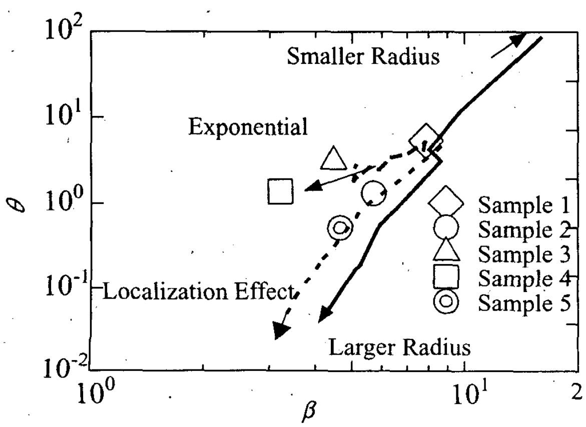

Fig. 7 The θ - β plots of the Weibull distributions measured for 5 samples reported in Ref. [7] and those simulated with three effects employed in this study. The growth conditions were for Sample 1: 10% diluted O_2 at 900 °C, Sample 2: O_2 + 5' anneal in N_2O, Sample 3: O_2 + 15' anneal in N_2O, Sample 4: O_2 + 30' anneal in N_2O, and Sample 5: 100% N_2O at 950 °C. Oxide thickness was 7 nm. Using this θ - β plot of the Weibull distribution, the cause of the change in breakdown statistics in a sample can be easily understood. In this case, the exponential effect and the localization effect must be considered.