Physical Modeling of Time Dependent Dielectric Breakdown (TDDB) of BEOL Oxide using Monte Carlo Particle Simulation

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***Abstract*—A simulation method for the TDDB of the BEOL oxide is investigated based on the 3D particle Monte Carlo simulation model which can evaluate the random motion of Cu ions in the oxide. While the conventional models do not consider the percolation theory of the TDDB phenomenon, the new model is based on the percolation model so that more rigorous physics can be considered. Also, the new method enables the statistical analysis of TDDB for the BEOL oxide. From the simulation study, it turns out that the assumptions of the previous models result in inaccurate characteristics and mechanisms. We expect that the simulation framework proposed in this paper could not only lead us to deeper physical insights but also could be readily applied to predict the reliability under the realistic conditions of the interconnect such as the 3D damascene structures or Cu-liner systems and so on.**

***Index Terms*—Back-End-Of-Line (BEOL) oxide, Time Dependent Dielectric Breakdown (TDDB), Monte Carlo simulation, Interconnect, Percolation theory**

I. Introduction

As the device technology node becomes continuously scaled down, the reliability of the Cu/low-k/Cu interconnect system, which is widely used as a Beck-End-Of-Line(BEOL) process, is considered as one of the limiting factor for further integration [1]–[5]. Especially, Time Dependent Dielectric Breakdown (TDDB) of the BEOL oxide, which is triggered by the injection of Cu^+ ions into the BEOL oxide, is one of the critical issue of the interconnect reliability [1]–[4], [6]. Therefore, theoretical modeling of the TDDB of BEOL oxide is required for understanding the physics and predicting the lifetime of the interconnects for the present and next technology node.

However, a main drawback of the conventional models [1], [2] is that the criterion for the oxide breakdown is assumed to be the point when the concentration of Cu^+ at the cathode reaches a certain critical value. Thus, models using such a “critical density criterion” may mislead the TDDB prediction since the “percolation” model, which is the underlying physical picture of the oxide breakdown [7], [8], is not included [3]. In addition, they can only predict the average value of the breakdown time (t_{BD}) without information on its distribution.

TABLE I
Comparison between BEOL oxide TDDB models.

	Hwang [2]	Chen [1]	This work
Criterion for breakdown	Density at cathode	Density at cathode	Percolation model
Statistical analysis	no	no	yes
Dimension	1D	1D	3D
Transport model of Cu^+	Drift and diffusion	Diffusion only	Drift and diffusion

For comparison between the previous and our model, we summarize key aspects of them in Table I.

The Authors have introduced a simulation framework using 3D Monte Carlo (MC) particle simulation for the TDDB simulation of BEOL oxide [9]. In this paper, we investigated a proposed simulation framework for calculating t_{BD} of BEOL oxide and its statistical properties. Since this model is based on the particle MC, the percolation path formation by Cu^+ particles could be naturally considered in evaluating t_{BD} with statistical information. With the simulation results, we discussed about the role of Cu transport and trap generation on the TDDB characteristics of BEOL oxide with more rigorous physical pictures.

II. Monte Carlo Simulation Method for Cu^+ induced TDDB

For the simulation, the following steps are considered within one simulation time step for the TDDB model: 1) Calculate the discrete position of each Cu^+ particle in the BEOL oxide according to the applied stress time. 2) Obtain the discrete position of the traps responsible for the breakdown. 3) Check whether the percolation path from the anode to the cathode is present or not (The percolation path is made up by TDDB traps). More details and the flowchart of the simulation can be found in elsewhere [9]. Here, we will review the simulation method [9]–[11] for reader’s convenience.

For the first step, We calculate all the trajectories of each Cu^+ particle by adopting the Langevin equation [12] that

describes the Brownian motion of the particle in 3D space as

$$\frac{du}{dt} = -\Gamma u + A(t) + K/m \tag{1}$$

where u is a velocity, m is a mass of the particle, A represents the white noise and K is a local electric field. In the above equation, Γ is a dynamical friction which can be written as

$$\Gamma = \frac{k_B T}{mD} \tag{2}$$

where D is the diffusion constant of the particle. The local electric field (K) changes due to the distribution of the Cu^+ particle and is updated for every time step by solving the Poisson equation.

In order to solve (1), Chandrasekhar [12] derived equations which can be used for MC simulations. The derivation can be successfully adopted for many systems including the mixed particle MC simulation on the semiconductor problems [13] and oxide degradation problems of MOSFET device [10], [11]. Here, we follow Chandrasekhar's derivation with notations in [13] to solve the position and velocity of the copper particle in the BEOL oxide if the initial values of the position (x_0) and velocity (u_0) at time t_0 are given. For 1D case, the position and the velocity at $t = t_0 + \Delta t$, are described as follows [12], [13]:

$$x = x_0 + \Gamma^{-1}(1 - e^{-\Gamma \Delta t})(u_0 - \frac{K}{\Gamma}) + \frac{K}{\Gamma}\Delta t + \sigma_x \omega_1 \tag{3}$$

$$u = u_0 e^{-\Gamma \Delta t} + \frac{K}{\Gamma}(1 - e^{-\Gamma \Delta t}) + x\sigma_u \omega_1 + \sigma_{u|x}\omega_2 \tag{4}$$

where

$$\sigma_x = F^{1/2}, \sigma_u = G^{1/2}, \sigma_{u|x} = G^{1/2}(1 - \frac{H^2}{GF})^{1/2} \tag{5}$$

and F, G and H can be written as follows:

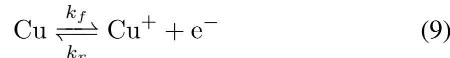
$$F = \alpha\Gamma^{-3}(2\Gamma\Delta t - 3 + 4e^{-\Gamma\Delta t} - e^{-2\Gamma\Delta t}) \tag{6}$$

$$G = \alpha\Gamma^{-1}(1 - e^{-2\Gamma\Delta t}) \tag{7}$$

$$H = \alpha\Gamma^{-2}(1 - e^{-\Gamma\Delta t})^2 \tag{8}$$

In the above equations, ω_1 and ω_2 are Gaussian random variables with unit variance so that $x(t)$ and $u(t)$ are determined stochastically. The equations described above can be easily extended to the 3D space with six independent Gaussian random variables.

The chemical process of the Cu injection at the anode interface between Cu electrode and oxide is known to be somewhat complicated [14]. In this simulation, we assumed that all the process of Cu ionization and injection can be represented by the following reaction equation



$$\mathrm{Cu} \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \mathrm{Cu}^+ + \mathrm{e}^- \tag{9}$$

After solving above equations, the spatial profile of the Cu^+ particles can be obtained for each time step as shown in Fig. 1.

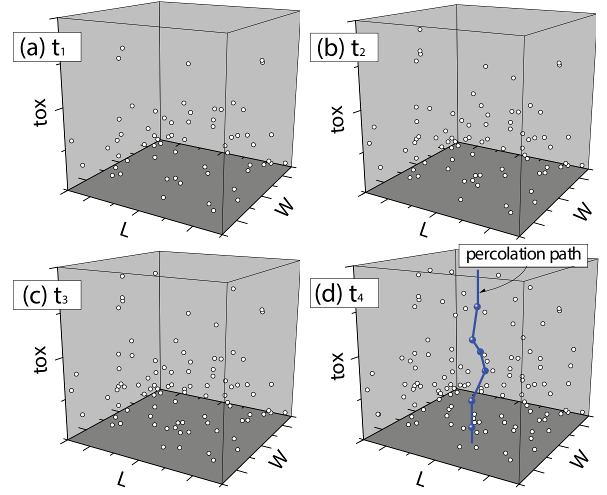


Fig. 1. Spatial profile of diffusing particles in a sample device under the influence of an electric field ($t_1 < t_2 < t_3 < t_4$). For each time step, the drift-diffusion of the particle and the presence of percolation path is calculated. Figure (d) shows the moment when the percolation path is generated.

For the second step, the position of the trap responsible for the TDDB is obtained based on the profile from step 1) as shown in Fig. 1. Some authors speculate that the nonbridging oxygen (NBO) atoms is generated by the Cu^+ ions and this may serve as the TDDB trap (Cu-induced trap model) [15]. However, there are no clear explanation on the form of the TDDB trap. Besides, the previous TDDB models of BEOL oxide assumes implicitly that the Cu^+ ion serves as the TDDB trap. Hence, we firstly investigated the assumption that Cu^+ itself is an active TDDB trap (Cu-trap model). After that, we have compared the Cu-trap model with the Cu-induced trap model.

For the third step, we make a judgement whether the percolation path is formed or not. Once the percolation path of Cu^+ is formed as shown with blue line in Fig. 1 (d), the oxide breakdown occurs. To reduce the simulation time, we used the k-d tree data structure for saving coordinates of Cu ions and the dijikstra algorithm [16] for the path finding from the anode to cathode. Since this is $O(NlogN)$ algorithm, the simulation time is reduced compared to the brute-force method which is $O(N!)$ algorithm.

III. Simulation Results

The Weibull plot of t_{BD} under various electrical field is shown in Fig. 2 calculated by the above mentioned method. We used identical 100 parallel capacitors with the length of 100nm, the width of 100nm and the thickness of 30nm. The simulation result follows the Weibull distribution similar to the experimental results (straight line in Weibull plot).

From the data in Fig. 2, the field dependence of the t_{BD} is depicted in Fig. 3. Also, the simulation result from Hwang, et al [2] is shown in Fig. 3. It is interesting point that the field dependence obeys the power-law (E^n) if the percolation model is considered while Hwang's calculation shows the $\sqrt{E}$

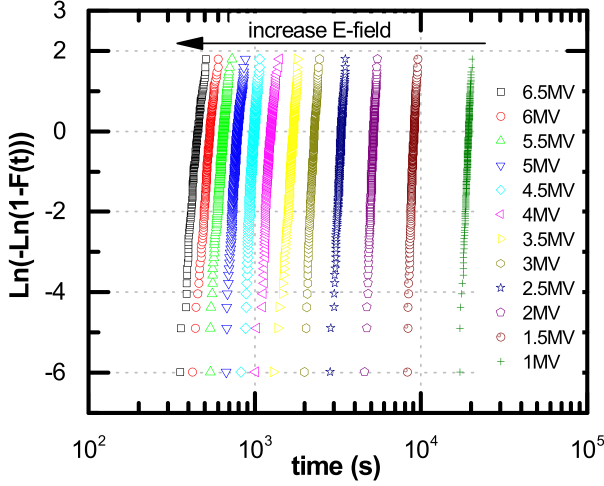


Fig. 2. Weibull plot of breakdown time calculated by 3D MC simulation for TDDB of BEOL oxide under various electric field (1MV/cm-6.5MV/cm).

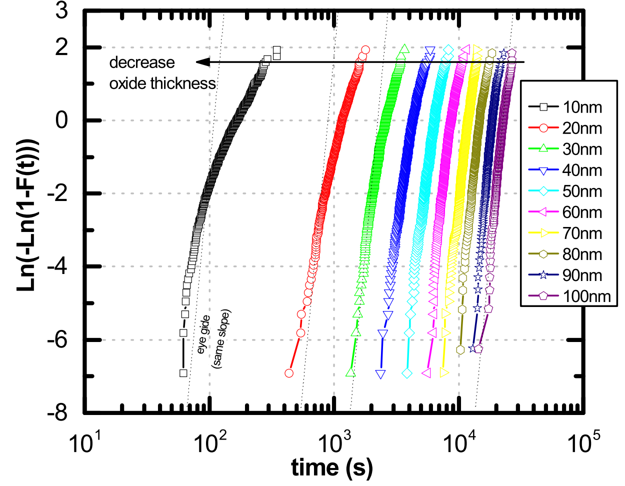


Fig. 4. Weibull plot of breakdown time calculated by 3D MC simulation for TDDB of BEOL oxide under various oxide thickness (10nm-100nm).

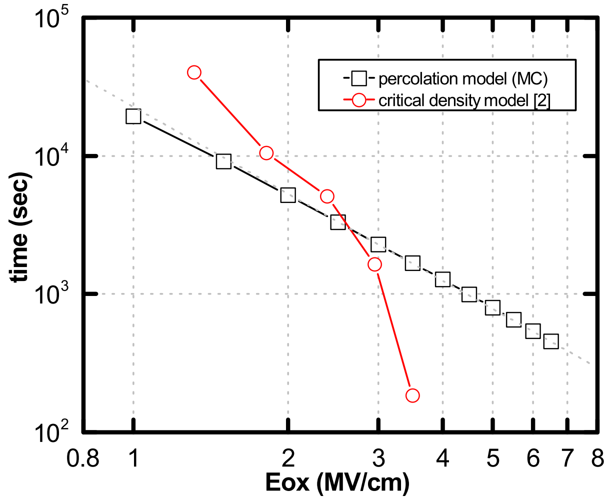


Fig. 3. Field dependence of the breakdown time (63.2% failure) under TDDB stress. After inclusion of the percolation model, the field dependence follows the power-law.

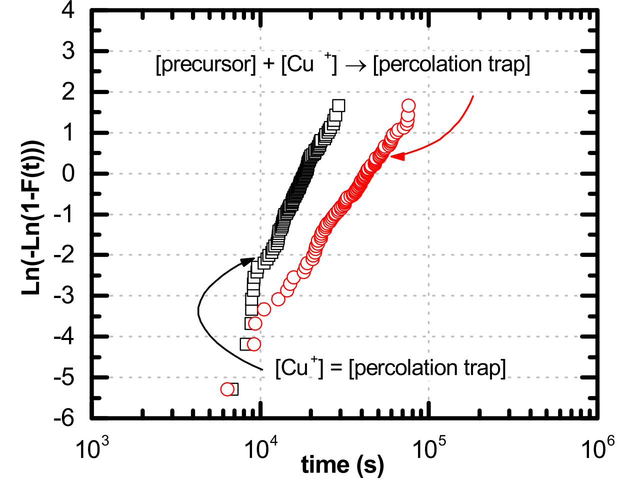


Fig. 5. Weibull plot for different definition of a percolation trap. If the percolation trap is assumed to be generated after the reaction of precursor and Cu^+, the distribution of t_{BD} becomes wider.

dependence [2]. Since other physical models such as drift-diffusion and boundary conditions are same for both calculations (refer TABLE I), it can be inferred that the conventional "critical density criterion" does not reflect the "percolation" nature of TDDB phenomenon. About the measurement result on the field dependence of the breakdown time, there are controversial arguments because some experimental results show $\sqrt{E}$ dependence [2], [6], [17] but others show power-law model [18], [19]. Only our theoretical approach which includes "percolation" nature gives a power-law model thus we expect that our MC methodology may give a hint to resolve the controversy.

The thickness dependence of the t_{BD} is also calculated as shown in Fig. 4. As the oxide thickness decreases, the average of t_{BD} is reduced following the power-law dependence. The increase of the distribution is also observed, which is a unique capability of our MC simulation framework.

It should be noticed that the distribution of t_{BD} predicted by the simulation is too narrow compared to the measurement results [1], [2], [18]. Interestingly, after the inclusion of the rate equation of new trap generation induced by Cu^+ (such as nonbridging oxygen [15]), the distribution becomes wider as shown in Fig. 5. Hence, it seems that that statistical analysis is crucial since the statistical parameter may reflect key physical mechanisms of the BEOL oxide breakdown.

IV. Conclusion

In order to model the TDDB of the BEOL oxide, we adopt the 3D MC method coupled with percolation model. It turns out that the assumptions of the previous models, without considering the percolation model, results in inappropriate characteristics and mechanisms so that our approach may resolve some controversy in the field dependence model [1],

[18]. Also, we found that the appropriate conversion mechanism from the diffusing Cu^+ to the active TDDB trap should be considered in order to predict accurate statistical properties.

The potential of the proposed simulation framework can be summarized as two folds: Firstly, it could be used to study the physical mechanisms of BEOL oxide breakdown so that it can resolve some controversies in the measurements [1], [18]. Secondly, we expect that this simulation framework can be readily used for the practical analysis considering real device characteristics such as the 3D damascene structures [20], the Cu-liner systems and porosity of low-k dielectrics and so on.

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References

[1] F. Chen, F. Ungar, A. H. Fischer, J. Gill, A. Chinthakindi, T. Goebel, M. Shinosky, D. Coolbaugh, V. Ramachandran, and Y. K. Siew, "Reliability characterization of BEOL vertical natural capacitor using copper and low-k SiCOH dielectric for 65nm RF and mixed-signal applications," *presented at the Int. Reliab. Phys. Symp., IEEE*, 2006, pp. 490495.

[2] S.-S. Hwang, S.-Y. Jung, and Y.-C. Joo,"The electric field dependence of Cu migration induced dielectric failure in interlayer dielectric for integrated circuits," *J. Appl. Phys.*, vol. 101, no. 7, pp. 074501, 2007.

[3] G. S. Haase, "An alternativemodel for interconnect low-k dielectric lifetime dependence on voltage," *presented at the Int. Reliab. Phys. Symp., IEEE*, 2008, pp. 556565.

[4] C.-C. Chen, M. Bashir, L. Milor, D. H. Kim, and S. K. Lim, "Backend dielectric chip reliability simulator for complex interconnect geometries," *presented at the Int. Reliab. Phys. Symp., IEEE*, 2012, pp. BD.4.1BD.4.8.

[5] M. Haurylau, G. Chen, H. Chen, J. Zhang, N. A. Nelson, D. H. Albonesi, E. G. Friedman, and P. M. Fauchet, "On-Chip Optical Interconnect Roadmap: Challenges and Critical Directions," *IEEE J. of Selected Topics in Quantum Electronics*, vol. 12, no. 6, 2006.

[6] F. Chen, O. Bravo, K. Chanda, P. McLaughlin, T. Sullivan, J. Gill, J. Lloyd, R. Kontra, and J. Aitken, "A comprehensive study of low-k SiCOH TDDB phenomena and its reliability lifetime model development," *presented at the Int. Reliab. Phys. Symp., IEEE*, 2006, pp. 4653.

[7] J. Sune, I. Placencia, N. Barniol, E. Farris, F. Martin, and X. Aymerich, "On the Breakdown Statistics of Very Thin SiO2 Films," *Thin Solid Films*, vol. 185, pp. 347-362, 1990.

[8] J. H. Stathis, "Percolation models for gate oxide breakdown," *J. Appl. Phys.*, vol. 86, pp. 5757, 1999.

[9] S. Choi, and Y. J. Park, "3D Monte Carlo Reaction-Diffusion Simulation Framework to model Time Dependent Dielectric Breakdown in BEOL Oxide"' *presented at the 11th Int. Workshop on Compact Modeling (IWCM)*, 2014.

[10] S. Choi, C.-K. Baek, S. Park, and Y. J. Park, "An Improved 3D Monte Carlo Simulation of Reaction Diffusion Model for Accurate Prediction on the NBTI Stress/Relaxation," *presented at the Int. Conf. on Simulation of Semiconductor Processes and Devices (SISPAD)*, Denver, USA, 2012, pp. 185-188.

[11] S. Choi, C.-K. Baek, S. Park, and Y. J. Park, "Stochastic Simulation of the NBTI and FN Relaxation using the 3D Monte Carlo Method," *presented at the 9th Int. Workshop on Compact Modeling (IWCM)*, Sydney, Austrailia, January 30, 2012.

[12] S. Chandrasekhar, "Stochastic Problems in Physics and Astronomy," *Rev. Mod. Phys.*, vol. 15, no. 1, pp. 1-89, 1943.

[13] G. Y. Jin, Y. J. Park, and H. S. Min, "Mixed particle Monte Carlo method for deep submicron semiconductor device simulator," *Trans. on Computer-Aided Design of Integrated Circuits and Systems*, vol. 10, no. 12, pp. 1534-1541, 1991.

[14] R. Achanta, W. N. Gill, J. L. Plawsky, and G. Haase, "Role of reactive surface oxygen in causing enhanced copper ionization in a low-k polymer," *J. Vacuum Sci. Tec. B*, vol. 24, pp. 1417, 2006.

[15] G. Barbottin, and A. Vapaille, "Instabilities in Silicon Devices: Silicon Passivation and Related Instabilities," *North-Holland*, Amsterdam, pp. 133, 1986.

[16] Pawan Jindal, Amit Kumar, and Shishir kumer, "Analysis of shortest path algorithms," *Global J. of Computer Sci. and Tech.*, vol. 10, no. 8, 2010.

[17] N. Suzumura, S. Yamamoto, D. Kodama, K. Makabe, J. Komori, E. Murakami, S. Maegawa, and K. Kubota, "A new TDDB degradation model based on Cu ion drift in Cu interconnect dielectrics," *presented at the Int. Reliab. Phys. Symp.*, 2006, pp. 484489.

[18] K. Croes, and Z. Tkei, "E- and E-model too conservative to describe low field time dependent dielectric breakdown," *presented at the Int. Reliab. Phys. Symp., IEEE*, 2010, pp. 543548.

[19] K. Croes, M. Pantouvaki, L. Carbonell, L. Zhao, G. P. Beyer, and Z. Tokei, "Comparison between intrinsic and integrated reliability properties of low-k materials," *presented at the Int. Reliab. Phys. Symp., IEEE*, 2011, p. 2.

[20] J. Gambino, F. Chen, and J. He, "Copper interconnect technology for the 32 nm node and beyond," *presented at the Custom Integrated Circuits Conf.*, 2009, pp. 141148.