Numerical Simulation of Percolation Model for Time Dependent Dielectric Breakdown (TDDB) under Non-uniform Trap Distribution

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***Abstract*—We propose a TDDB model which can predict the breakdown time distributions when the trap distribution in the oxide is "non-uniform". This is an extension of the conventional cell-based model that has been limited to the case of uniform trap distribution. The verification of the proposed model is conducted by comparing it with the Monte Carlo simulation. It turns out that the proposed model successfully reproduce the MC simulation result for various trap profiles including the cases of a high-K gate stack and a BEOL oxide. Since the model can be coupled with more realistic trap generation models, more accurate predictions based on the rigorous physics may possible including the percolation theory and oxide degradation models.**

***Index Terms*—TDDB, Cell based model, Monte Carlo simulation, BEOL oxide, high-K gate dielectric, Non-uniform trap distribution**

I. Introduction

A cell-based model [1], which has an analytic form, has been widely used for predicting the breakdown time distribution of TDDB. The physical background of the cell-based model is solid because it is based on the percolation theory which is a physical origin of TDDB. The model has been mostly applied to the case of "uniform" trap profile in space, yet has not been tested for that of "non-uniform" trap. One of such non-uniform cases, for example, is a high-K (HK) interfacial layer (IL) gate stack because the trap generation rates for HK and IL layer are different [2]. Another important case is an extrinsic failure [1] which is caused by an external particle injection, for example, in a BEOL oxide by Cu^+ injection [3], [4].

As a solution for the extrinsic TDDB of the BEOL oxides, the critical density model (CDM) has been sometimes used [3], [4]. However, since only the average trap density [4] or a local trap density [3] is considered by CDM, it may not reflect the percolation theory [1], [5]. The Monte Carlo (MC) method [2], [5] can be a physically rigorous solution for above problems. In the MC method, the defect sites (traps) are randomly distribution in the oxide, and then the formation of a percolation path is calculated. However, even though the MC method is an accurate solution for TDDB, it always requires a lot of simulation costs.

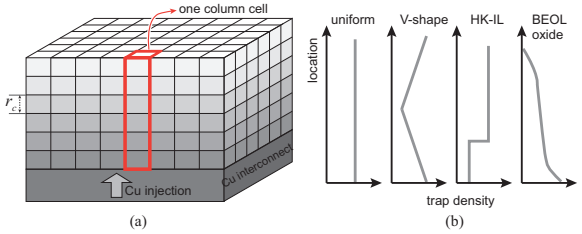

Fig. 1. (a) Schematics of the 3D cell-based simulation model for a TDDB simulation. Each cell has a non-uniform trap density (represented by gray level) in a vertical direction. For the BEOL oxides, Cu ions are injected from the Cu interconnect (cathode) and it gives rise to the non-uniform Cu trap distribution. The breakdown probability for one column cell is firstly evaluated using (1) and then the failure probability for entire region is calculated using (2). (b) Trap density profiles along the thickness direction used in this study: a uniform distribution, a V-shape distribution and distributions from the HK-IL gate stack and the BEOL oxide.

In this work, we propose an analytic Percolation Theory based TDDB Model (PTM) for the non-uniform trap distribution. This is an extension of the cell-based model for the non-uniform case and it can be coupled with equations describing the spatial trap generation models. The validation of the PTM is conducted by comparing it with MC results. The calculations are conducted with various kinds of trap profiles and the critical distances (r_c). Here, the critical distance is defined as a maximum distance between the two traps to make a conduction path and is a key parameter in percolation theory [1]. In addition, PTM is coupled with Cu^+ transport equations in the BEOL oxide and compared with the CDM.

II. PTM for Non-uniform Traps

A conventional analytic model, the cell-based model [1], calculates the probability for failure of one column cell (F_{col}) in Fig. 1 with a uniform trap density. Since the size of one cell is same as the critical distance (r_c), the failure of one column cell means that the percolation path is formed from the bottom to the top electrodes in Fig. 1(a).

If we consider the non-uniform trap density, the failure probability of each cell is different according to the defect or trap density. Hence, F_{col} should consider the spatial and

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time variation of trap density and can be written as

$$F_{col} = \prod_{i=1}^{m} \langle \lambda(ir_c, t) \rangle \tag{1}$$

where $m = t_{ox}/r_c$ and $\langle \lambda(x,t) \rangle$ is an average trap number in one cell. If $\langle \lambda(x,t) \rangle$ is less than 1, $\langle \lambda(x,t) \rangle$ is same as a probability to finding one trap in the cell or equivalently, a failure probability of the cell.

According to the cell-based model, the failure probability for entire area (F) can be written as,

$$F = 1 - (1 - F_{col})^N \tag{2}$$

where $N = LW/r_c^2$. Hence, when substitute (1) into (2), the F becomes

$$F(t) = 1 - (1 - \prod_{i=1}^{m} \langle \lambda(ir_c, t) \rangle)^N \tag{3}$$

and the spatial trap density is considered in the above equation. So, once the trap density profile is given, the failure rate can be evaluated numerically using (3).

For the extrinsic failure, the trap distribution can be obtained from the transport and reaction of injected particles. The transport equation of metal (Cu^+) is solved to model TDDB of the BEOL oxide. The transport equation considers the drift and diffusion term under the electric field and can be written as [6]

$$F(x) = -ba \cosh\left(\frac{\partial C}{\partial x}\right) + 2bC \sinh\left(\frac{qaE}{2kT}\right) \tag{4}$$

where b is $\nu a^2 e^{-qW/kT}$, ν is the frequency of attempted jumps, a is the hopping distance, W is a height of the potential barrier, C is a concentration of Cu^+ and E is an applied electric field. Since the charged copper ion is responsible for the TDDB of BEOL oxide, the Poisson equation is coupled with (4) as [3], [5].

The equations to obtain the Cu^+ profile in the BEOL oxide under the electric field stress is same with the previous work [3]. However, in calculating the failure probability from the Cu^+ profile, our method uses (3) based on PTM while the previous work [3], based on CDM, assumes that the average breakdown time is proportional to the time when the following condition is satisfied;

$$C(t_{ox}, t) = \langle \lambda(t_{ox}, t) \rangle / r_c^3 = C_{critical} \tag{5}$$

where t_{ox} is a oxide thickness, $C_{critical}$ is a critical concentration for breakdown and the Cu^+ is injected at $x = 0$. The difference between results using PTM with (3) and CDM with (5) is compared in Chapter IV.

III. Validation of Proposed Model

The results from (3) of the PTM are compared with the MC results for a model validation under various oxide trap profiles as shown in Fig. 1(b): 1) uniform trap distribution, 2) V-shape trap distribution, 3) HK-IL gate stack and 4) BEOL oxide (in Chapter IV). For the MC simulation, the traps are randomly distributed according to the each profile in Fig. 1(b) and the number of samples that has a percolation path is counted. In this work, number of samples for each MC simulation is 10^5.

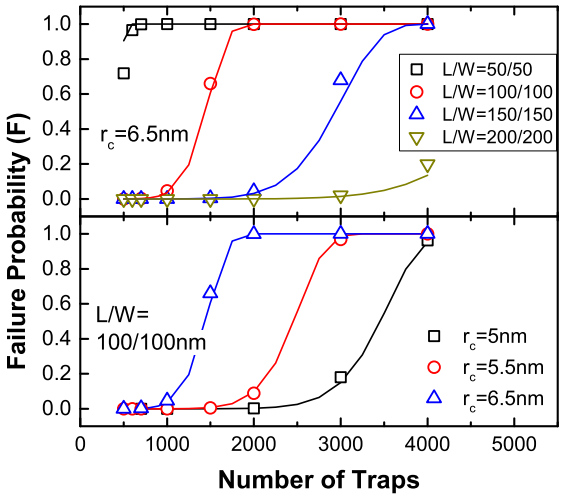

Fig. 2. CDF of t_{BD} for uniformly distributed traps calculated by MC (symbols) and PTM (lines) under (a) various areas and (b) critical distances. $L/W/t_{ox}$ of oxide is 100/100/40nm.

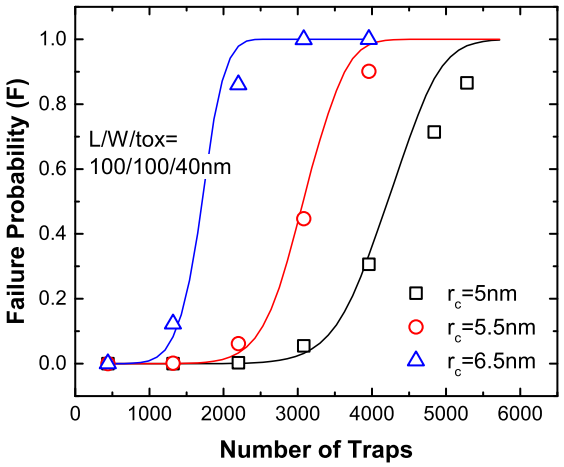

Fig. 3. CDF of t_{BD} for V-shape distributed traps calculated by MC (symbols) and PTM (lines) under various critical distances. The dimension of oxide ($L/W/t_{ox}$) is 100/100/40nm.

The calculated failure probability of samples that has a uniform profile is shown in Fig. 2. In the figure, the result using both the MC method (symbols) and PTM (lines) are shown. Since PTM is same as the conventional cell-based model in this case, both results are well matched as shown in Fig. 2 for various area and critical distances.

The failure probability is also evaluated for the distribution with V-shape function as shown in Fig. 3. Interestingly, it can be verified that the results of analytic equations (line) are well matched with that of MC (symbol) method not only for the uniform traps but also for the non-uniform traps. Also, the PTM successfully reproduces the dependence of r_c as shown

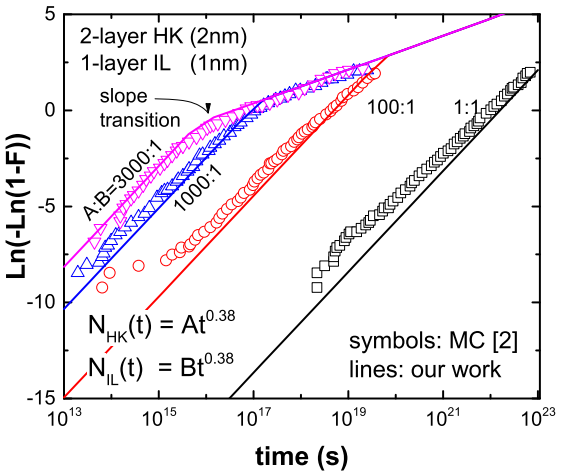

Fig. 4. Weibull plot of HK-IL layers calculated by MC (symbols) [2] and PTM (lines) with various ratios of the trap generation rate between HK and IL. (HK:IL = 1:1-3000:1)

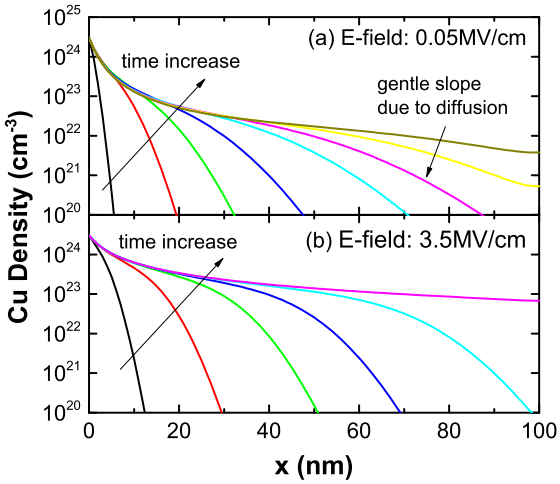

Fig. 5. Spatial profile of Cu^+ ions in the BEOL oxide with a 100nm thickness under the E-field of (a) 0.05MV/cm and (b) 3.5MV/cm. Simulation parameters for Cu transport is adopted from [3].

in Fig. 3.

In the HK-IL gate stacks, a trap distribution shows a step function as shown in Fig. 1(b). This is because that the trap generation rate of HK oxide is higher than that of IL oxide. T. Nigam, *et al* has studied TDDB characteristics of the HK-IL gate stacks using both experimental and simulation ways [2]. The experimental result shows that there are a transition in the Weibull slope and the MC simulation result reveals that this transition arises due to the different trap generation between HK and IL oxides. They used a power-law model for the trap generation which can be written as

$$N(t) = Gt^{0.38} \tag{6}$$

where G is a trap generation rate. Various ratios of the generation rate for HK and IL oxide (G_{HK}:G_{IL}=3000:1-1:1) are used for the simulation and the Weibull distribution of the breakdown time from the MC simulation conducted by T. Nigam, *et al* is shown in Fig. 4 with symbols (data is from Fig. 6 in [2]). For our PTM simulation on the HK-IL stacks, trap generation model and parameters are same as that of [2].

The simulation results using our analytic PTM equation in (3) for the HK-IL oxide are shown with lines in Fig. 4 together with MC result in [2] for various ratios of trap generation rate (G) between HK and IL. It is interesting point that our model well reproduces the MC simulation results including the transition of Weibull slope and the dependence on G_t.

IV. BEOL OXIDE TDDB

A Cu^+ profile in the BEOL oxide is calculated using (4) for each time steps as shown in Fig. 5. Since the diffusing particle is charged, (4) is coupled with Poisson equation. Well-tuned parameters from [3] are used for the simulation. The Fig. 5 shows the Cu^+ profiles of both low field (0.05MV/cm) and a high field regime (3.5MV/cm). Since the diffusion component is more dominant in the low field regime, the Cu profile

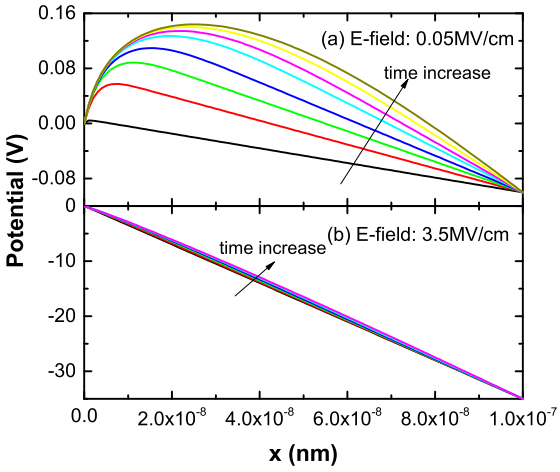

Fig. 6. Potential profile of the BEOL oxide under the electric field of (a) 0.05MV/cm and (b) 3.5MV/cm. Because of the change in Cu^+ profile, the potential profile changes as the stress time.

shows more gentile slope (shown in Fig. 5(a)) than that in the high field regime (Fig. 5(b)). The variation of the electrostatic potential due to the change of Cu distribution, as shown in Fig. 6, is considered for the simulation.

From the Cu^+ profile, the probability for breakdown is calculated using both (3) (lines) and MC method (symbols) as shown in Fig. 7 with different r_c. The analytic results with (3) well reproduce the MC results.

The Weibull plot of t_{BD} under various E-field is shown in Fig. 8. An interesting point is that the slope decreases in the low E-field regime, consistent to the trend from measurements [7]. This is due to the transition from a drift regime (high field) to a diffusion regime (low field), and the effect of diffusion can be confirmed by the gentler slope of Cu profile in low field regime (Fig. 5(a)). Since the shapes of Cu profile are different

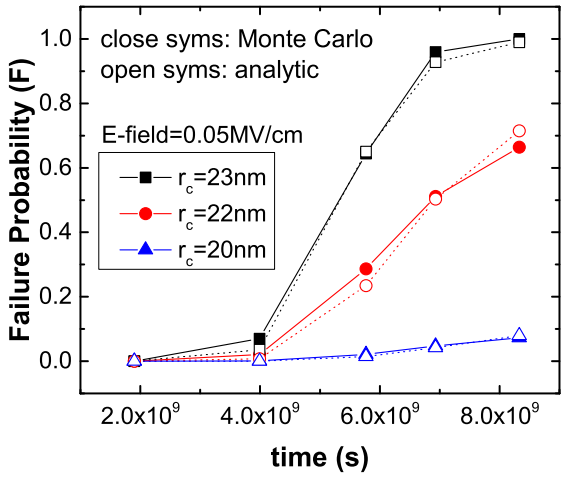

Fig. 7. Failure Probability of t_{BD} for the BEOL oxide using the Cu profile as in Fig. 5 with various r_c. Applied E-field is 0.05MV/cm and calculation is done by MC (symbols) [5] and our analytic model (lines).

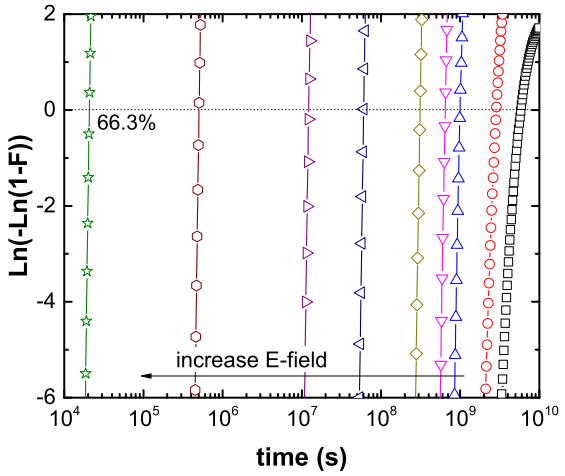

Fig. 8. Weibull plot of t_{BD} for the BEOL oxide for various E-fields (0.05MV/cm-3.50MV/cm). PTM is used for the simulation.

in high and low field regime, the different characteristics in F are predicted according to (3).

In this context, it is worthwhile to mention that our model reflects the information of trap profile while CDM neglects the information because CDM considers the trap density of just one points or an average density as (5). Hence, CDM cannot reflect the slope transition in Fig. 9 and shows different field dependence in the low field region as shown in Fig. 9. Thus, it can be inferred that the CDM for BEOL oxide [3] could fail to reflect the percolation nature of TDDB phenomenon.

V. Conclusion

We propose an analytic TDDB simulation model for the oxide with a non-uniform trap distribution. Comparison studies with MC are conducted and the proposed model can successfully applied to several situations with non-uniform trap

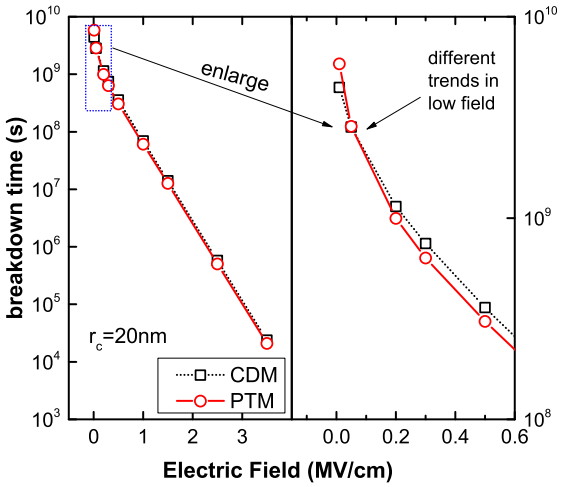

Fig. 9. Field dependence of t_{BD} for 66.3% breakdown in Weibull plot calculated by CDM (square symbols) and PTM (circle symbols). The left graph enlarges the low field regime.

profiles including the high-K gate stacks and BEOL oxides. This model can efficiently capture the percolation theory, a basic physical picture of TDDB, with low simulation costs unlike CDM [3] or MC method [2], [5]. Since PTM can be coupled with more realistic trap generation models as demonstrated with BEOL oxide, we expect that more accurate predictions based on the rigorous physics is possible.

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