Temperature- and voltage-dependent trap generation model in high-k metal gate MOS device with percolation simulation*

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High-k metal gate stacks are being used to suppress the gate leakage due to tunneling for sub-45 nm technology nodes. The reliability of thin dielectric films becomes a limitation to device manufacturing, especially to the breakdown characteristic. In this work, a breakdown simulator based on a percolation model and the kinetic Monte Carlo method is set up, and the intrinsic relation between time to breakdown and trap generation rate R is studied by TDDB simulation. It is found that all degradation factors, such as trap generation rate time exponent m, Weibull slope β and percolation factor s, each could be expressed as a function of trap density time exponent α. Based on the percolation relation and power law lifetime projection, a temperature related trap generation model is proposed. The validity of this model is confirmed by comparing with experiment results. For other device and material conditions, the percolation relation provides a new way to study the relationship between trap generation and lifetime projection.

Keywords: high-k metal gate, TDDB, percolation theory, kinetic Monte Carlo, trap generation model

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1. Introduction

High-k metal gate stacks are being used to suppress the gate leakage due to tunneling for sub-45 nm technology nodes.[1–3] Multi-layer gate dielectric of the high-k/interfacial layer (HK/IL) brings not only promising performance but also reliability challenges. Especially for sub-1-nm equivalent oxide thickness (EOT) metal oxide semiconductor (MOS) devices, the reliability of thin dielectric film becomes a limitation to device manufacturing.[4–6]

For thin dielectric, the breakdown characteristic is no longer the same as classical electric field (E-field) driven phenomenon. A number of studies suggest that the trap generation in oxide is the main cause for final breakdown.[7–9] The breakdown events are related to the trap generation process and percolation path formation. For a lifetime projection model, a universal power law model is obtained over wide ranges of EOT and stress voltage.[10,11] It is evident that different models yield drastically different lifetime results in affecting the specification supply voltage.

The percolation theory has proved that the distribution of breakdown events is an intrinsic mechanism.[8] By using Monte Carlo (MC) simulation, the area scaling law and Weibull distribution are obtained, and the decrease of Weibull slope with reducing oxide thickness is well explained. Furthermore, with an application of the kinetic Monte Carlo (kMC) method, bimodal Weibull distribution of TDDB is explained as different trap generation rates in high-k and interfacial layer.[9]

In this work, based on the percolation model and the kinetic Monte Carlo (kMC) method, a simulator of the breakdown process is set up. The intrinsic relation between time to breakdown and trap generation rate R is studied by simulations. The degradation factors each are written as a function of trap density time exponent α. By combining the percolation relation with power law lifetime projection, a temperature related trap generation model is proposed to study the dielectric degradation. It is found that the generated trap is thermally activated, with the activation energy being about 0.11 eV. For different device and material conditions, the trap generation process could also be connected with the breakdown characteristic by the percolation relation.

2. Experiment

MOS capacitors are fabricated as follows. Firstly, Si wafer with a resistivity of 2 Ω ∼ 4 Ω for n-type is cleaned by diluted buffered oxide etch solution. Then the interfacial layer is formed by ozone oxidation. The HfO_2 layer is deposited by atom layer deposition (ALD) with about 2.4-nm-thick used as the high-k dielectric. Continuously, post annealing at 450 °C is treated. Then a 2-nm-thick TiN and a 1-nm-thick TaN layer are formed by ALD, and a 3-nm-thick TiN layer by chemi-

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cal vapor deposition (CVD). Finally, 75-nm-thick W layer are deposited as gate electrode.

All electric measurements are performed by an Agilent 4155B and 4294A. The temperature in measurement ranges from 25 °C to 125 °C. MOS capacitors are stressed in the accumulation area for constant voltage stress (CVS) and ramp voltage stress (RVS). The areas under test are all 100 μm^2. The EOT of gate stacks is about 1.07 nm and the physical thickness of HfO_2 is about 2.4 nm. An abrupt increase of gate current is used as the failure criterion and the current after breakdown is about 2 mA.

3. Percolation relation between initial trap generation rate R_0 and T_{BD}

3.1. Percolation model simulation

Percolation model simulations are conducted based on the kMC method on a three-dimensional (3D) cubic grid. The dielectric is divided into 100×100 cells in the plane of the substrate and 3-to-6 layers of dielectric. Thus, the edge effect is negligible. For each set of simulations, 64-1000 breakdown events are recorded to fit the experiment results. The flowchart of the simulation is shown in Fig. 1.

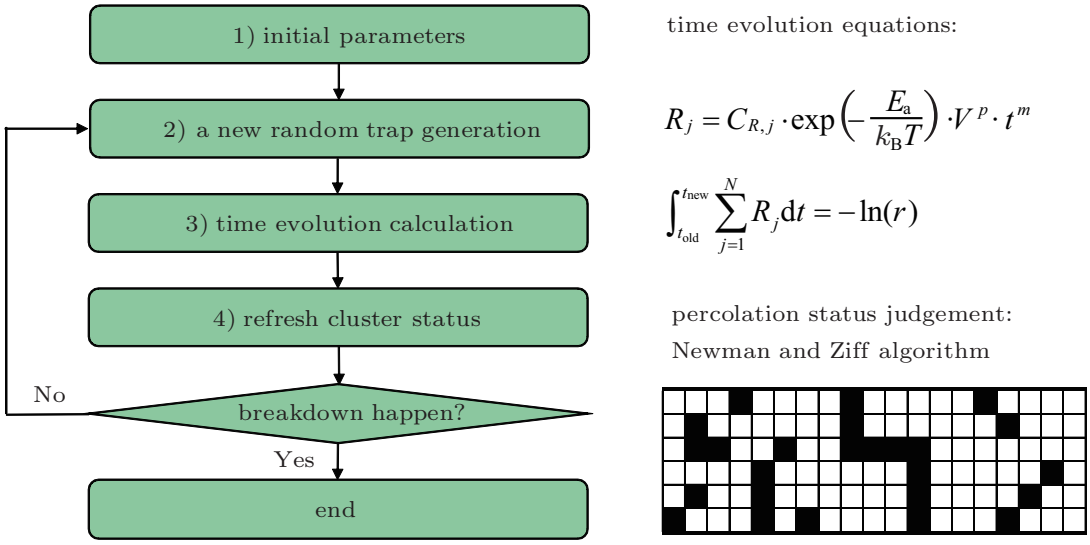


Fig. 1. (color online) Flowchart of percolation simulation and percolation diagram in 2D mode.

In each simulated step, a new trap is generated in a random site and time evolves in a random increment influenced by the time dependent trap generation rate. When a percolation path connecting two interfaces, the breakdown event is recorded.

In this work, the trap density time exponent $\alpha = 0.38$ is used according to Ref. [9]. Then, 6 of the total dielectric layers could be used in simulation due to a constant experiment Weibull slope of about 2.3. Then the gate dielectric is treated as a 4-layer high-k + 2 layer IL and the trap effect distance $a_0 = 6$ Å. The trap generation rates of high-k and IL are treated as the same value due to the single Weibull distribution in this work. The Weibull distribution of simulation results is normalized based on the Poisson area scaling law to an experiment test area.

3.2. Trap generation rate in simulations

The trap generation rate R in each cell is defined as follows:

$$R = R_0 \cdot t^m, \tag{1}$$

where R_0 is the initial trap generation rate, and m is the time exponent factor. It is assumed that the initial trap generation rate R_0 is dependent on the stress condition. This trap generation rate expression is consistent with the power relation of the trap generation process in stress induced leakage current (SILC) or bias temperature instability (BTI) measurement.[11–13]

Based on the above trap generation rate, the relation between T_{BD} (time to breakdown) and initial trap generation rate R_0 could be studied by simulation. The trap generation rate time exponent m is set to be −0.62 according to trap density time exponent α.

The simulation results by varying initial trap generation rate are shown in Fig. 2, and the relation between T_{BD} and R_0 could be expressed as

$$T_{BD} = C_{TR} \cdot R_0^{-s}, \tag{2}$$

where s is the positive power exponent and defined as the percolation factor, and independent of dielectric thickness. It is indicated that with a higher initial trap generation rate, the breakdown happens in less time.

Based on the above results, it is concluded that s is independent of dielectric thickness and only dependent on degradation factor m. It is the result of an intrinsic characteristic of percolation theory and independent of lifetime projection and

statistics. Thus, s could be regarded as a degradation factor. The percolation factor is also a useful parameter to connect percolation simulation and lifetime projection.

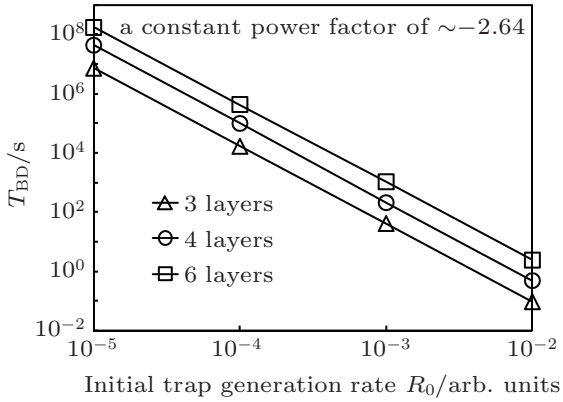


Fig. 2. Plots of simulated T_{BD} versus initial trap generation rate R_0. A constant power exponent factor $-s$ is independent of dielectric thickness.

3.3. Degradation factors in percolation model

Here, a detailed study is given to describe the relation of degradation factors. All degradation parameters are useful to study the dielectric degradation process, including trap density time exponent α, trap generation rate time exponent m, Weibull slope β and percolation factor s.

Firstly, α is the time exponent factor of trap density, as shown below

$$N_{OT} = N_0 \cdot t^{\alpha}. \tag{3}$$

This trap generation rate is similar to the power relation of the trap generation process in SILC or BTI measurements. It is indicated that trap density increases with stress time increasing. The trap generation rate is defined as the derivative of N_{ot} with respect to time:

$$R = \frac{dN_{ot}}{dt} = R_0 \cdot t^{m}, \tag{4}$$

where $m = \alpha - 1$ is the power exponent of time. Owing to the fact that α is always in a range from 0.3 to 0.4, m is a negative value. It is concluded that the trap generation rate decreases as stress time is increasing.

Based on the above discussion, α and m are physical parameters related to the trap generation process during stress tests. The other two parameters s and β are simulation factors in the percolation model simulation.

The Weibull slope β is one of the simulation degradation factors. The value of Weibull slope describes the spreading characteristic of T_{BD} distribution. The relation of β is obtained from simulation results (Fig. 3) and consistent with previous results reported in other work[14,15]

$$\beta = \alpha \cdot \frac{T_{ox}}{a_0}, \tag{5}$$

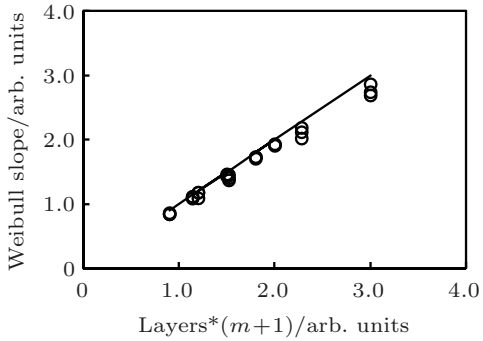


Fig. 3. Relation between Weibull slope β and α.

Finally, the percolation factor s in the percolation relation is also studied in the relation with α. An intrinsic relation between s and α is obtained below and shown in Fig. 4,

$$s = \frac{1}{\alpha}. \tag{6}$$

This relation is an empirical result, and well consistent at α values ranging from 0.1 to 0.9 as shown in Fig. 4. It is proved that s is also a degradation factor and strongly dependent on the trap generation process.

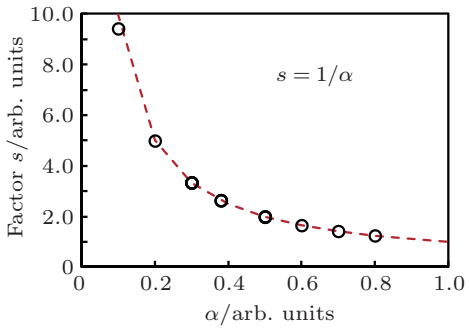


Fig. 4. (color online) Relation between percolation factor s and α.

As a conclusion, with percolation model simulation, all degradation factors could be expressed as functions of trap density time exponent α. All these parameters are related to the trap generation process and dielectric breakdown. These parameters are useful in reliability assessment and lifetime projection.

4. Temperature- and voltage-dependent trap generation model

4.1. Lifetime projection model

Temperature related model is significant for the in-depth understanding of the trap generation process. In TDDB measurements, stress voltages are from 2.7 V to 3.2 V and temperatures are set to be 25 °C, 60 °C, 90 °C, and 125 °C, respectively. Under each measurement condition, 11–20 devices are tested for truncated statistic analysis and the Weibull distributions for test results are shown in Fig. 5. The Weibull slope is treated as a constant value ~ 2.3 and independent of stress. It is noted that the solid lines in Fig. 5 are only guide lines for $\beta \sim 2.3$ and not the fitting results.

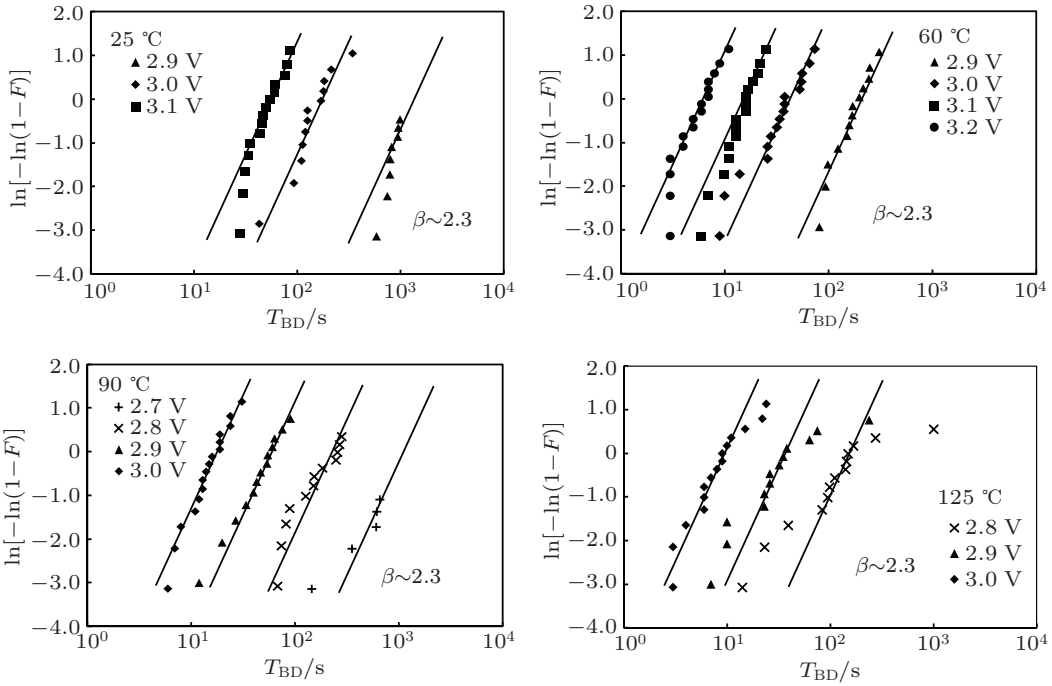


Fig. 5. TDDB results under different stress conditions.

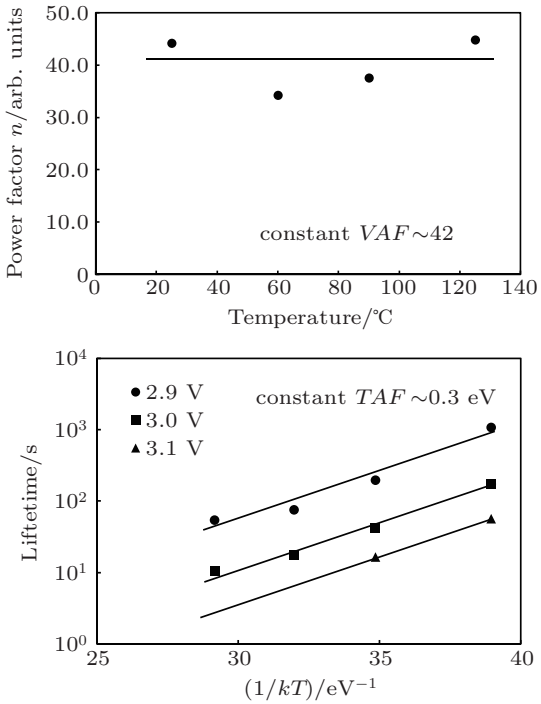


Fig. 6. *VAF* and *TAF* dependence under different stress conditions.

Based on $T_{\rm BD}$ extracted from the above TDDB results, a temperature related power law model is proposed for lifetime projection. It could be written as

$$\begin{aligned} T_{\rm BD} &= C_{\rm T}\exp\left(\frac{H}{kT}\right)V^{-n},\\ VAF &= -\frac{\partial \ln T_{\rm BD}}{\partial \ln V} = n,\\ TAF &= k\frac{\partial \ln T_{\rm BD}}{\partial (1/T)} = H. \end{aligned} \tag{7}$$

From the experimental results in Fig. 6, the *VAF* (short for voltage acceleration factor) is about 42 and the effective activation energy of breakdown is about 0.3 eV in this paper. Note that due to only 3 or 4 points are used for fitting, there appear more errors in the determintion of *VAF*. However, it is a reasonable assumption that *VAF* is temperature-independent.[16,17] The effective activation energy is related to the thermal activation energy of the generated trap and shows the saturation at high temperature (higher than 125 °C). Thus the *TAF* (short for temperature acceleration factor) is extracted from room temperature to 125 °C.

4.2. Trap generation model

Based on the above lifetime projection model and percolation relation, combining Eqs. (1), (2), and (7), the trap generation model is proposed as follows:

$$\begin{aligned} R &= \left(\frac{C_{\rm TV}}{C_{\rm TA}}\right)^{-1/s}\cdot\exp\left(-\frac{H}{sk_{\rm B}T}\right)\cdot V^{n/s}\cdot t^{m}\\ &= C_{\rm R}\cdot\exp\left(-\frac{E_{\rm a}}{k_{\rm B}T}\right)\cdot V^{p}\cdot t^{m}, \end{aligned} \tag{8}$$

where $C_{\rm R}$ is a constant pre-factor, $E_{\rm a} = H/s$ is the activation energy of the generated trap, and the power factor $p = n/s$. Using this model instead of Eq. (1) in the percolation simulation, the stress condition dependent $T_{\rm BD}$ is obtained. The simulation results are well consistent with the experimental results as shown in Fig. 7.

This model indicates that the trap generation is a thermal activation process and the activation energy of the generated trap is about 0.11 eV in this paper. The activation energy and

voltage power law factor of the generated trap could be obtained from *VAF* and *TAF* in the lifetime projection and percolation factor *s*.

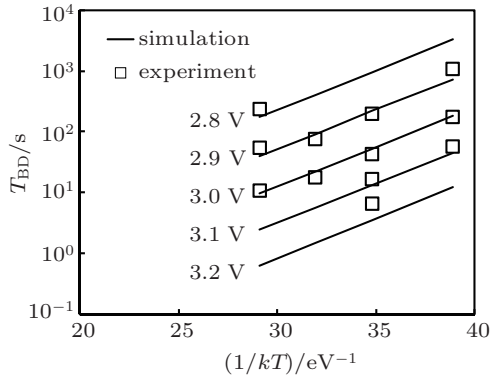


Fig. 7. Experimental and simulation results for different stress conditions.

From the above results, the trap generation model is determined by the lifetime projection and percolation relation. For other conditions, lifetime projection models are different, especially for temperature dependence.[16–18] Thus, for different materials and devices, the trap generation model should be corrected with the lifetime projection model and percolation relation. The trap activation energy E_a could be obtained from the *TAF* and percolation factor *s* for different materials.

5. Conclusions

In this work, a temperature and voltage dependent trap generation model is proposed. It is useful for TDDB simulation and lifetime projection in reliability assessment. A simulator of the breakdown process is set up based on the percolation model and the kMC method. The intrinsic relation between T_{BD} and initial trap generation rate R_0 is obtained from simulation results. The power exponent *s* is defined as the percolation factor due to the intrinsic percolation relation. Four degradation related factors could be unified as functions of trap density time exponent α. By combining the percolation relation with the power law model, the temperature and voltage dependent trap generation model is obtained. It is found that the trap generation process is a thermal activation process, with the activation energy being 0.11 eV. The power exponent and activation energy of trap generation are correlated with the *VAF*, *TAF* in the power law model and percolation factor *s*. A good correlation with experimental results confirms the validity of this model. This model is applicable in percolation model simulation and provides a new way to study the trap generation process and lifetime projection. For other device and material conditions, the trap generation process could be related to the lifetime projection model through the percolation relation.

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