# An Improved 3D Monte Carlo Simulation of Reaction Diffusion Model for Accurate Prediction on the NBTI Stress/Relaxation

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***Abstract*—We developed the 3D Monte Carlo simulation framework for the Reaction Diffusion model of NBTI. For the first time, we report that the RD model can predict the experimental features of NBTI stress/relaxation when the microscopic properties are considered in 3D space such as the capture cross-section, density and reaction energy of Si-H bonds. We expect that our simulation framework would be effectively used for the accurate prediction of trap generation/relaxation in general semiconductor/insulator systems.**

***Index Terms*—NBTI, Reaction Diffusion model, Monte Carlo Simulation, Relaxation Characteristics, Discrete trap, Langevin equation**

## I. Introduction

Negative Bias Temperature Instability (NBTI) is one of the most serious challenges in the scaled VLSI devices [1]. The Reaction Diffusion (RD) model was widely used for the prediction of the interface trap generation under NBTI after its first proposal in 1977 [2]. However, it has been seriously criticized because of its inaccuracy in predicting the fast measurement results on relaxation phases [3], [4], making the NBTI model highly controversial until now [4], [5]. Therefore, it is worthwhile to verify the competing models for NBTI in order to rule out such controversies. In this context, we investigate recent arguments [5] on the RD model in order to study the validity of the model by proposing an advanced simulation framework.

The "failure" of the conventional RD model [4], [6], [7] is described in Fig. 1. In the figure, the universal fitting [6] from the RD model is shown with the own measurement data. The problem is that the 50% of the interface trap is recovered at the point where the stress time is same as the relaxation time while the actual measurement results show much less recovery. Moreover, the recovery is completed in $\sim$6 decades according to RD model but the actual recovery is slower.

So far, tuning of any parameters of the RD model could not resolve the problems shown in Fig. 1. Recently, the effective diffusion constant has been speculated in the relaxation phase to resolve the problem on the RD model [5]. According to the speculation [5], H should laterally diffuse (hover) in order to find the unsaturated Si- bond for recombination as described in Fig. 2. Since the diffusing trajectory become lager due to the lateral diffusion, the effective diffusion constant for the recovery phase becomes smaller resulting in the slower recovery. In order to justify this speculation, some authors tried a stochastic simulation in a 2D space using equally spaced dangling bonds but every attempt have been failed to correct the relaxation behavior [8], [9]. In this work, we develop a 3D Monte Carlo Reaction Diffusion (MCRD) framework as suggested by the authors [10] and conduct the stochastic NBTI simulation to consider the random nature of the $Si/SiO_2$ interface without spatial discretization. Contrary to the previous work [8], [9], we could observe that the lateral diffusion is naturally included. With our 3D-MCRD framework, we demonstrate that the RD framework can accurately predict both NBTI stress/relaxation phases.

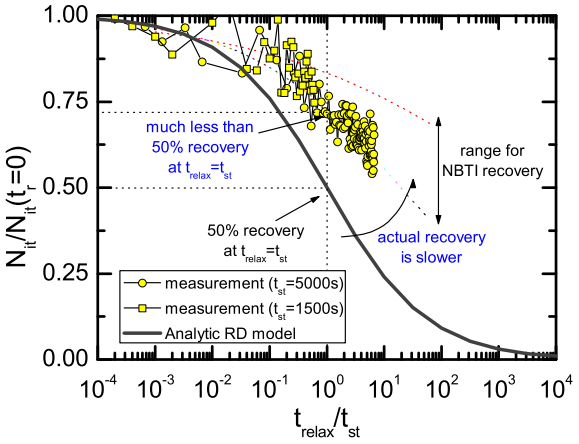


Fig. 1. NBTI relaxation phase where the data is scaled by the universal relaxation law [6]. The measurement result (symbols) are much slower than the simulation result of the analytic RD model (solid line). For measurement data, the Subthreshold Swing method is used to extract the interface trap density. The range for NBTI recovery reported by the literatures are also shown.



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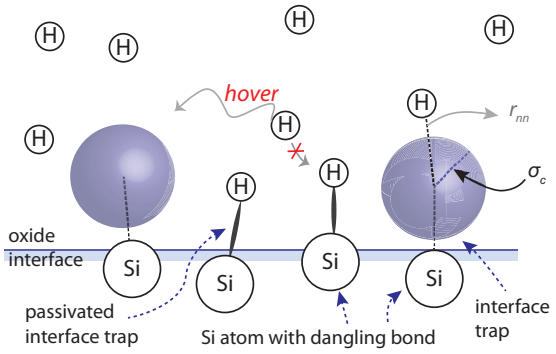


Fig. 2. Schematic representation of the $Si/SiO_2$ interface. The trajectory of H becomes longer than the 1D case because hydrogen have to find unsaturated Si- bond, making the effective diffusion constant becomes smaller.

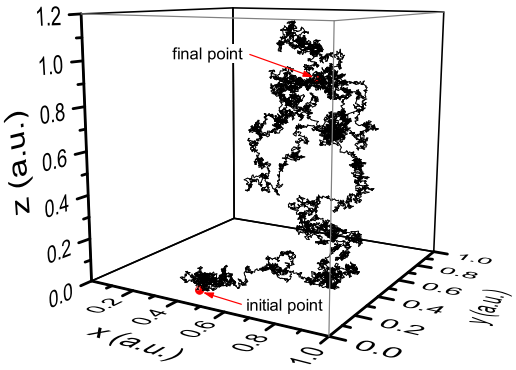


Fig. 3. The trajectory of a sample particle in the 3D space, calculated by the Langevin equation (1). The Brownian motion of the hydrogen particle is observed.

## II. 3D MCRD Model

In order to trace the trajectory of each H particle, we adopt the Langevin equation [11] which describes the Brownian motion of the particle in a 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, $\Gamma$ 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, $k_B$ is the Boltzmann constant and $T$ is temperature.

In order to solve (1), Chandrasekhar [11] 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 [12]. We follow Chandrasekhar's derivation with notations in [12] to solve the position and velocity of the hydrogen particle in the 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 determined as follows [11], [12]:

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

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

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, $\omega_1$ and $\omega_2$ 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 case for our 3D MCRD model. The random 3D motion of a sample hydrogen particle is shown in Fig. 3 implemented by (3) and (4).

At the $Si/SiO_2$ interface, the Si-H bond can be dissociated or recovered by the following reaction:

$$\mathrm{Si{-}H} \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \mathrm{Si\cdot} + \mathrm{H} \tag{9}$$

The dissociation reaction probability ($k_f$) for each Si-H bond during $\Delta t$ is

$$k_f \Delta t = e_H \exp(E_f \cdot g(\sigma_f)/k_B T) \tag{10}$$

and the recovery reaction probability ($k_r$) during $\Delta t$ is

$$k_r \Delta t = C_H U(\sigma_c - r_{nn}) \exp(E_r \cdot g(\sigma_r)/k_B T) \tag{11}$$

where $e_H$ is a dissociation constant, $C_H$ is a recovery constant, $r_{nn}$ is the distance between H and unsaturated Si bond, $\sigma_c$ is the capture cross-section of the unsaturated Si bond, $U$ is a unit step function, $E_f$ and $E_r$ are activation energies for the reactions and $g$ is the Fermi-derivative function which can represent the Gaussian distribution with variance $\sigma_c$ and $\sigma_r$.

In summary, the RD equations [2], [5] are solved by the MC method in 3D using (3) and (4) for diffusion; (10) and (11) for reaction at the interface to obtain the interface trap number ($N_{it}$).

## III. Simulation Result

We conduct the 3D MCRD simulation for NBTI and observe the behaviors of individual random traps as shown in Fig. 4. For the Monte Carlo simulation, the number of particles is fixed to 5000 and the area of device is scaled according to the given Si-H density. The hydrogen atoms ($H^0$) are assumed to be diffuse out while the hydrogen molecules ($H_2$) are actual diffusing species [5] [8]. Since the difference of the H and $H_2$ model gives a slightly different result in stress phase only [5],

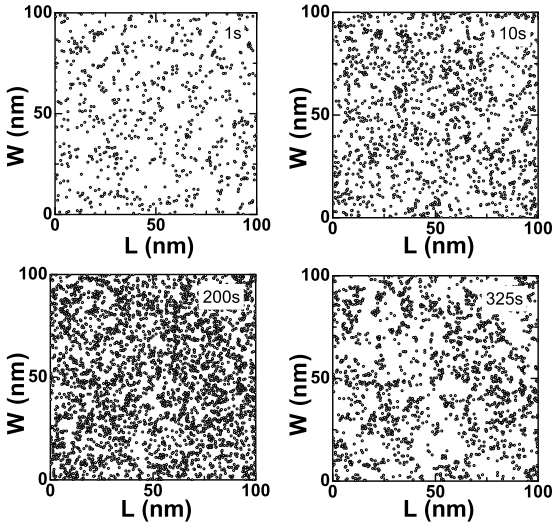


Fig. 4. 2D discrete distribution of the interface trap under NBTI stress (1, 10, 200s) and relaxation phase (325s).

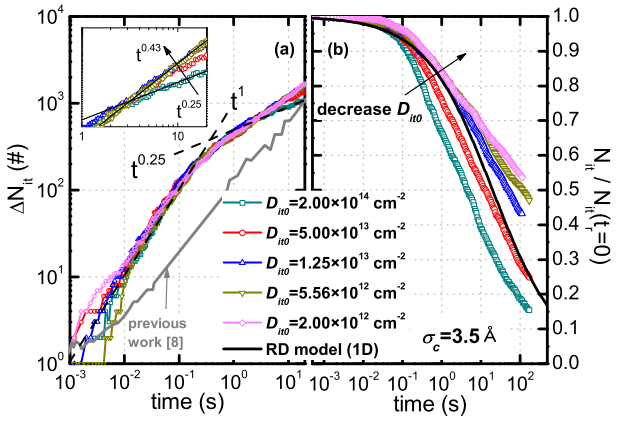


Fig. 5. 3D MCRD simulation results for the stress phase (a) and the relaxation phase (b) with various $D_{it0}$.

the assumption does not distort the recovery behavior which is our main concern.

In order to demonstrate the correction of the 1D RD model, we investigate the effect of the total density of the Si- bond ($D_{it0}$) and the $\sigma_c$ in (11) which are expected to mostly affect to the lateral diffusion in terms of the average distance between Si- bonds and the free flight time of H, respectively.

The 3D MCRD simulation results on the stress and relaxation phase are shown in Fig. 5 with various $D_{it0}$ ($\sigma_c$ is set to 3.5 Å). We assume the homogeneous Si-H bonds ($\sigma_f = \sigma_r = 0eV$) same as the assumption in the conventional RD model. When $D_{it0}$ is $2.00 \times 10^{14} cm^{-2}$, the characteristic reaction limited region ($N_{it} \propto t^n$ with $n = 1$) and diffusion limited region ($n = 0.25$) are well reproduced by the 3D MCRD simulation in contrary to the previous attempt [8], [9] (refer Fig. 5(a)). Therefore, both the microscopic and the macroscopic model are consistent in $N_{it}$ for the NBTI stress

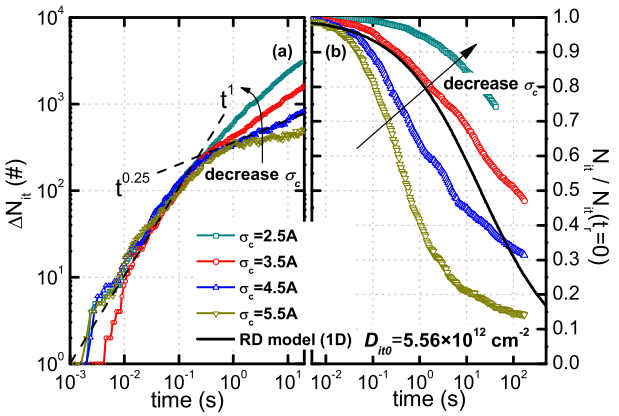


Fig. 6. 3D MCRD simulation results for the stress phase (a) and the relaxation phase (b) with various $\sigma_c$.

phase. Note that $n$ of 0.25 can be coverted to $n$ of 0.16 which is observed in experiments, when the $H_2$ is considered as diffusing species. Interestingly, as $D_{it0}$ decreases, the recovery becomes slower as shown in Fig. 5(b). When $D_{it0}$ is less than $1.25 \times 10^{13} cm^{-2}$, the recovery becomes slower than that predicted by the 1D RD model. It can be explained in terms of the average distance; as the $D_{it0}$ decreases, the average distance between Si-H bonding increases. Hence, the hydrogen particle should fly more to find the unsaturated Si- bond and thus the effective diffusion constant become smaller. In sum, an additional lateral diffusion is enhanced so that the recovery becomes slower as the $D_{it0}$ decreases. Notwithstanding the recovery behavior is in the reasonable range when $D_{it0}$ is less than $1.25 \times 10^{13} cm^{-2}$, the stress behavior becomes inconsistent ($n > 0.25$) under such range of $D_{it0}$ as shown in the inset of Fig. 5(a).

The simulation results with various $\sigma_c$ are shown in Fig. 6 under $D_{it0}$ of $5.56 \times 10^{12} cm^{-2}$. When $\sigma_c$ is smaller than 3.5Å, the recovery characteristics enter into the proper range. This is because the free flight time of hydrogen becomes longer so that the effective diffusion constant is again decreased. However, the reduction of $\sigma_c$ further increases $n$ in the stress phase which is contrary to the experimental observation. To sum up, the 3D MCRD simulation with the homogeneous Si-H bond reveals the followings; 1) As the speculation in [5], the lateral diffusion do affect to the recovery characteristics. 2) the recovery speed of the RD model are influenced by the microscopic parameters such as $D_{it}$ and $\sigma_c$. 3) Even though the recovery can be corrected, there is no combination of $D_{it}$ and $\sigma_c$ which satisfy the experimental features of both stress and relaxation phases.

Now, the inhomogeneity in Si-H bonds [13] in (10) and (11) ($\sigma_f = 0.06eV$, $\sigma_r = 0.07eV$) are considered for the 3D MCRD simulation and data for $N_{it}$ with various $D_{it0}$ and $\sigma_c$ are shown in Fig. 7 and Fig. 8, respectively. For all the conditions of $D_{it0}$ and $\sigma_c$, we found that the slower relaxation followed by the appropriate stress behavior ($n \sim 0.25$), which agrees well with the criteria of both stress/relaxation phases

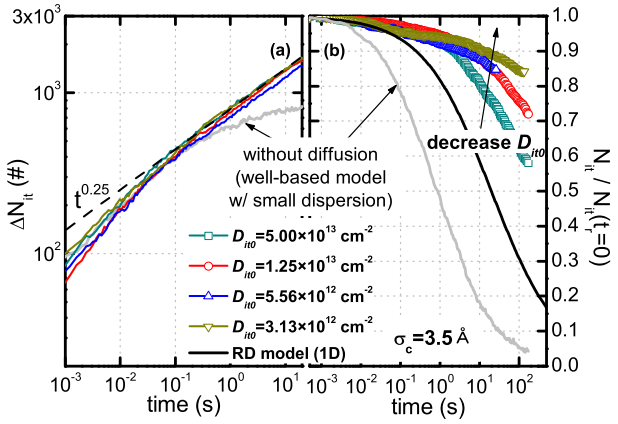


Fig. 7. 3D MCRD simulation results for the stress phase (a) and the relaxation phase (b) with various $D_{it0}$. The dispersion of the reaction energy are considered as $\sigma_f = 0.06eV$ in (10) and $\sigma_r = 0.07eV$ in (11).

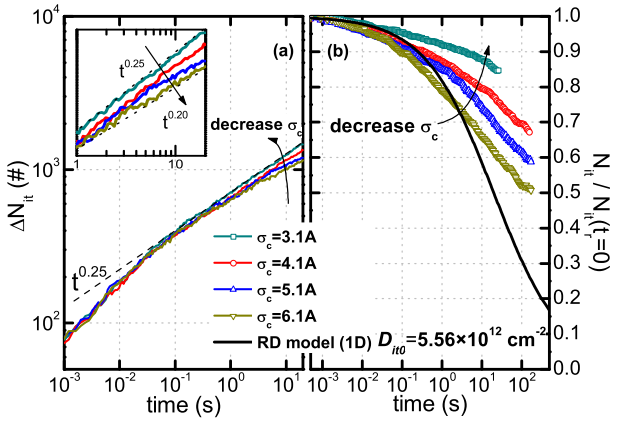


Fig. 8. 3D MCRD simulation results for the stress phase (a) and the relaxation phase (b) with various $\sigma_c$. The dispersion of the reaction energy are considered as $\sigma_f = 0.06eV$ in (10), $\sigma_r = 0.07eV$ in (11).

(refer Fig. 1). This is in contrast to the well-based model [4] (an alternative model for NBTI) which cannot reproduce the features on the interface trap with reasonable values [5], [13] for $\sigma_f$ and $\sigma_r$ as shown in Fig. 7 by the gray line. Hence, it can be inferred that physics from competing NBTI models (the diffusion from RD model and the dispersion of reaction energy from well-based model) should be simultaneously considered for an accurate NBTI model covering the stress and relaxation phases.

## IV. Conclusion

In order to resolve the controversies on the RD model, we developed the 3D MCRD simulation framework which is a microscopic version of the analytic RD model. Since our MCRD framework can trace the motion and reaction of each hydrogen particle stochastically, we can verify the recently raised speculation on the RD model including the concept of lateral diffusion [5]. For the first time, we report that the RD model is indeed influenced by the lateral diffusion and the recovery behavior can be adjusted to fit the experimental features when $D_{it0}$ and $\sigma_c$ are considered. However, we cannot adjust the parameters of the MCRD model to explain both stress and relaxation phases properly, which means that the present form of the RD model is insufficient even if the lateral diffusion is considered. Interestingly, when the dispersion of reaction energy of Si-H bonds ($\sigma_f$ and $\sigma_r$) are considered, both stress and relaxation phases are accurately predicted under the MCRD framework. Our work calls more investigations to justify whether the 3D MCRD model can accurately predict the numerous data on NBTI including AC/DC, temperature, voltage dependencies, etc. We expect that the 3D MCRD simulation framework would be a vital tool for exploring the validity of the RD based model.

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