

# On the Microscopic Limit of the Modified Reaction-Diffusion Model for the Negative Bias Temperature Instability

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**Abstract**—It has recently been proposed that the inability of the reaction-diffusion model for the negative bias temperature instability to properly predict the experimentally observed recovery transients is due to the incomplete description of atomic motion in the one dimensional macroscopic formulation of the theory. In order to investigate this claim, we develop a microscopic formulation of the modified reaction-diffusion model and simulate it using the kinetic Monte Carlo algorithm. The results of the macroscopic and the atomistic formulation are compared. It shows that the recovery behavior predicted by the RD theory is not affected by the change of the formulation. However, differences arise for the degradation behavior, which, as the microscopic formulation is the physically more accurate description, raise questions regarding the physical relevance of the reaction-diffusion theory. In extension it is shown that any rate-equation based description in the atomic level context will be unable to properly describe the early stages of degradation.

## I. INTRODUCTION

The negative bias temperature instability (NBTI) is one of the most critical degradation effects observed in p-channel metal-oxide-semiconductor (pMOS) transistors. Since its suggestion in 1977, the reaction-diffusion (RD) model [1] has been the most popularized explanation for NBTI. The model assumes that hydrogen is released from the interface and subsequently diffuses into the bulk of the oxide. While the reaction at the interface is assumed to be fast and in quasi-equilibrium, it is the diffusion of the hydrogenic species which controls the degradation. During the last decade the model has gone through a number of refinement stages [2–4]. The current version assumes that long-term degradation and recovery is dominated by  $H_2$  diffusion. While this version of the RD model could successfully be calibrated to constant-bias degradation data, striking contradictions began to emerge when researchers started to look at the detailed features of recovery [5–12].

It has recently been speculated that the failure of the RD theory to explain the experimentally observed long relaxation tails could be due to the fact that the model uses macroscopic rate equations together with the solution of the one-dimensional diffusion equation [13]. The stochastic three-dimensional motion of the diffusing atoms has been suggested

to lead to a longer effective diffusion path than what is obtained from a one-dimensional diffusion model. According to the authors of [13], this could explain the experimentally observed long recovery tails, while leaving the degradation behavior unchanged. In their paper, they correct the one-dimensional RD model by including a reduced diffusion coefficient during recovery.

We have recently developed a microscopic stochastic formulation of the H-based RD theory to investigate these suggestions [14]. Our calculations showed that while this description leaves the recovery largely unchanged, the predicted degradation strongly deviates from the results of the classic RD model and the experimentally observed NBT degradation. In the present work, we extend our microscopic model to include molecular hydrogen and discuss the difference between the stochastic and the deterministic description of the problem.

## II. THE MICROSCOPIC RD MODEL

The modified RD model has been developed as an extension of the classical RD models, which assume an instantaneous transition between the liberated interfacial hydrogen and the diffusing species, usually  $H_2$  [13, 15–18]. It extends the previous models by explicitly treating H as well as  $H_2$  diffusion and interconversion between the two species.

The reactions present in the modified RD model are the interface reaction  $\text{Si-H} \rightleftharpoons \text{Si-}\bullet + \text{H}$ , the dimerization reaction  $2\text{H} \rightleftharpoons \text{H}_2$ , and the diffusion of both species. The mathematical framework is based on reaction rate equations of macroscopic densities [15, 16]

$$\frac{\partial N_{\text{it}}}{\partial t} = k_f(N_0 - N_{\text{it}}) - k_r N_{\text{it}} H_{\text{it}}, \quad (1)$$

$$\frac{\partial H}{\partial t} = -D\nabla^2 H - k_{\text{bond}} H^2 + k_{\text{break}} H_2, \quad (2)$$

$$\frac{\partial H_2}{\partial t} = -D_2 \nabla^2 H_2 + \frac{k_{\text{bond}}}{2} H^2 - \frac{k_{\text{break}}}{2} H_2, \quad (3)$$

where  $N_{\text{it}} = [\text{Si-}\bullet]$  is the interface state density,  $N_0 = [\text{Si-H}]_0$  the initial density of passivated interface defects,  $H_{\text{it}}$  the hydrogen concentration at the semiconductor-oxide

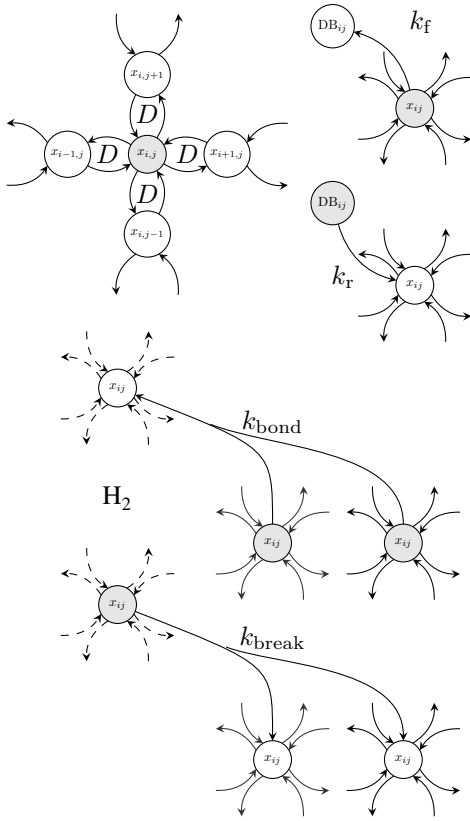


Fig. 1. Reaction channels available to the hydrogen atoms (occupancy is indicated by the gray fill). Within the bulk  $\text{SiO}_2$  (**top left**), the atoms or molecules are allowed to jump to all neighboring sites in the three-dimensional orthogonal grid with a constant hopping rate  $D$  or  $D_2$ , respectively. At the interface, some nodes also offer a bonded state to the hydrogen atom (**right top**). If a bonded state is already occupied the corresponding bonding reaction channel is removed. When two hydrogen atoms occupy the same interstitial position, they can undergo a dimerization at rate  $k_{\text{bond}}$  and form  $\text{H}_2$  (**bottom**). Each hydrogen molecule decays at a rate  $k_{\text{break}}$  back into two hydrogen atoms.

interface, while  $k_f$ ,  $k_r$ ,  $k_{\text{bond}}$ , and  $k_{\text{break}}$  are the reaction rates for depassivation, passivation, dimerization, and atomization, respectively. The motion of H and  $\text{H}_2$  is described by a simple diffusion law, where  $\text{H} = [\text{H}](x, t)$ ,  $\text{H}_2 = [\text{H}_2](x, t)$ , with the corresponding diffusion coefficients  $D$  and  $D_2$  [19].

The microscopic view of the modified RD model is established by tracing the macroscopic equations back to their elemental reactions. This also requires to replace the macroscopic quantities  $N_{\text{it}}$  and  $N_{0,\text{H}}$  and  $\text{H}_2$  by atomic actors, i.e. dangling bonds, hydrogen atoms and hydrogen molecules, all and each as separate entities. The atomic motion is then treated as hopping transport between interstitial sites, the passivation/depassivation and the dimerization/atomization reactions are treated as elemental reactions that are spatially localized inside an interstitial position (see Fig. 1). In the following, the interstitial sites are assumed to form a regular and orthogonal three-dimensional grid and the hopping rates  $D$  and  $D_2$  are assumed to be constant in accord with the isotropic and non-dispersive diffusion underlying the conventional macroscopic

RD model [15, 16, 20]. The distance between the interstitials is assumed to be  $4\text{\AA}$ , which corresponds well with calculations on atomistic silica models [21]. Additionally, a hopping rate of  $100\text{s}^{-1}$  is assumed for both H and  $\text{H}_2$ , leading to a macroscopic diffusion coefficient of  $1.6 \times 10^{-13}\text{cm}^2/\text{s}$ , which matches the parameters in [22]. Although in the real  $\text{SiO}_2$  of a MOS transistor the amorphous structure will lead to a random network of interstitial sites [21] with a variety of hopping rates and a more complex topology, these variations are assumed to be unimportant in the RD model [19].

The Si/SiO<sub>2</sub> interface is represented by an array of special interstitial sites at the bottom of the simulation box. The density of interface states used in macroscopic descriptions is realized by giving selected interface sites the ability to bond or release a diffusing hydrogen atom as illustrated in Fig. 1. For example, a typical  $N_0$  of  $10^{12}\text{cm}^{-2}$  [16, 23] can be modeled by selecting 16 interface interstitials of a simulation box with a lateral extension of  $100 \times 100$ . This corresponds to an average distance of the interfacial sites of 10nm.

### III. COMPUTATIONAL METHOD

As explained in the previous section, the actors of our RD system are restricted to a countable number of states as the macroscopic diffusion in a continuous space is replaced by a hopping between the metastable interstitial positions. It is worthwhile to note that this discretization is not a mathematical approximation but rather follows directly from the microscopic picture. It is now possible to define a state vector  $\vec{x}$  that contains the interstitial positions and bonding states of all actors as well as a set of reaction channels which cause transitions between the states of this vector. The RD system then becomes a time-dependent stochastic process  $\vec{X}(t)$  that exists in one of a countable set of states  $\vec{x}_i$ . According to the theory of stochastic chemical kinetics [24], the evolution of the system over time can then be described by a chemical master equation

$$\frac{\partial P(\vec{x}, t)}{\partial t} = \sum_{j=1}^M [a_j(\vec{x} - \vec{v}_j)P(\vec{x} - \vec{v}_j, t) - a_j(\vec{x})P(\vec{x}, t)], \quad (4)$$

where  $P(\vec{x}, t) = P(\vec{X} = \vec{x}, t | \vec{x}_0, t_0)$  is the probability that the stochastic process  $\vec{X}(t)$  equals  $\vec{x}$  at time  $t$ , given  $\vec{X}(t_0) = \vec{x}_0$ . The physics are contained in the propensity functions  $a_j$  and the state-change vectors  $\vec{v}_j$  for the  $M$  reaction channels. In our formulation, the propensity functions take very simple forms as explained in [14].

The thus formulated master equation is straight-forward to solve using the stochastic simulation algorithm (SSA) [24] explained in Fig. 2, which is also known as the kinetic Monte Carlo method. The SSA does not have any algorithmic parameters and is a mathematically exact description of the system defined by the states and reaction channels [24].

### IV. RESULTS

As shown in Fig. 3, a random three-dimensional motion of the diffusing hydrogen is obtained from this description as

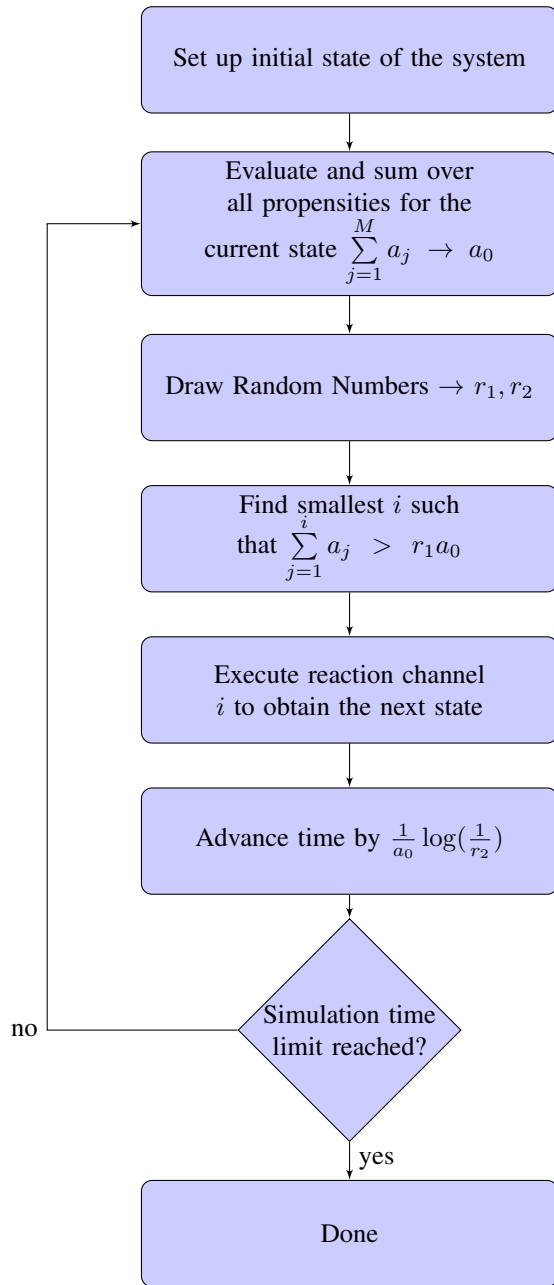


Fig. 2. Sketch of the stochastic simulation algorithm (SSA) [24] that was used to simulate the microscopic RD model. The algorithm generates a realization of the stochastic process described by the chemical master equation (4).

suggested in [13]. As in [14], all degradation and recovery calculations were performed on an ensemble of two-dimensional systems due to the lower computational demand. Nevertheless, our test-calculations in three dimensions have shown that all relevant effects are already present in a two-dimensional topology. The distance between two dangling bonds in our two dimensional model is 4nm (one dangling bond every 10 interstitials).

#### A. Lateral Equilibration

A typical degradation curve as generated by our RD implementation is displayed in Fig. 4. It shows that the degradation

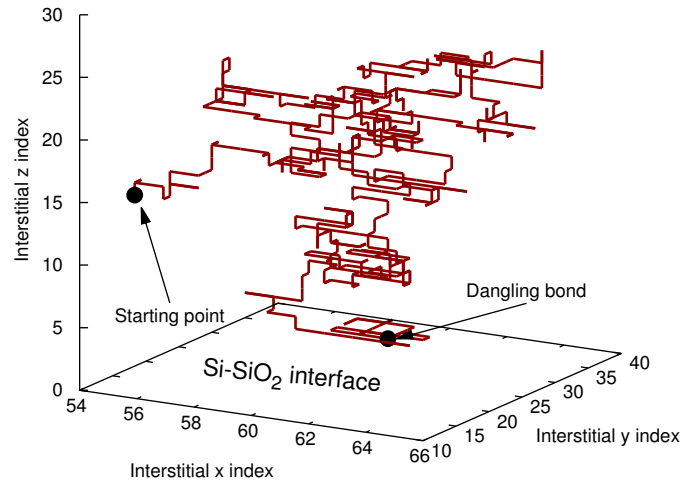


Fig. 3. Final part of the trajectory of a hydrogen atom in the atomic hydrogen microscopic RD model [14] during recovery calculated using the stochastic simulation algorithm (SSA). The motion clearly proceeds in a three-dimensional stochastic fashion as requested by [13].

behavior of the microscopic RD model strongly deviates from the macroscopic version, in accord with our previous work which didn't include hydrogen molecules [14]. Instead of the three regions which arise from the macroscopic RD model — reaction limited, intermediate plateau and diffusion-limited — the H-H<sub>2</sub> microscopic description shows five regimes.

- The earliest degradation times ( $t < 2 \times 10^{-5}$  s in this case) are dominated by the depassivation of dangling bonds. This regime is similar to the reaction-limited regime in macroscopic RD calculations.
- After the passivation and depassivation has reached an equilibrium between  $k_f$  and  $k_r$  separately for each Si–H bond, the fraction of depassivated dangling bonds remains constant until the diffusion of the hydrogen atoms becomes dominant.
- As more and more hydrogen atoms leave their initial position, the degradation is determined by the buildup of the diffusion front along the Si-SiO<sub>2</sub> interface and the equilibration between the dangling bonds. This regime is a direct consequence of the physical picture behind the RD theory and has a very large power-law exponent that is not experimentally observed. The stress time range in which this regime is observed depends on the average distance between two dangling bonds, the diffusion coefficient and the interstitial size.
- After a common diffusion front has formed, the diffusion-limited regime begins to emerge. However, as a sufficient amount of H<sub>2</sub> has not formed yet, the initial diffusion-limited regime has the typical  $t^{1/4}$ -form that arises from the hydrogen-atoms-based RD model [14].
- Eventually, for long degradation times the macroscopic H<sub>2</sub>-diffusion-limited behavior is obtained.

In the macroscopic RD models, the onset of the diffusion-limited regime only depends on the diffusion coefficient, which needs to establish a large enough flux of particles into the

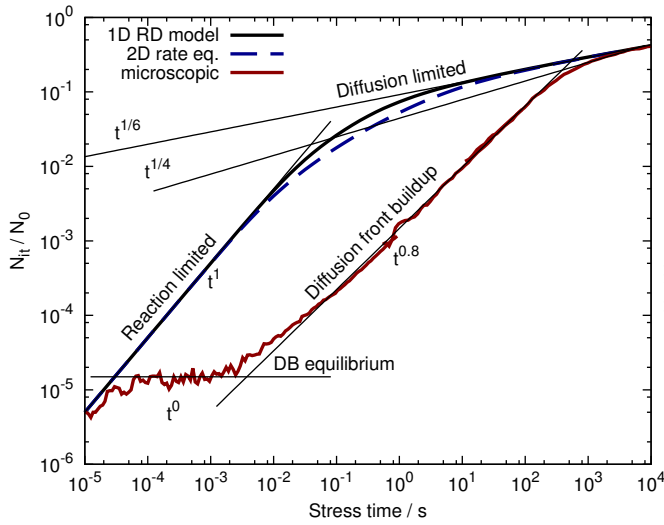


Fig. 4. A typical degradation transient as obtained by our microscopic RD implementation. Four main regimes can be defined, which are indicated in the figure. The microscopic result is compared to a calculation on a similar structure (simulation box with interface width 100 and oxide depth 1000, every tenth interface node is a dangling bond) and a rate-equation based description. Apart from a slight deviation in the transition from the reaction-limited to the diffusion-limited regime, the two-dimensional model with isolated dangling bonds follows the classical one-dimensional RD model.

oxide. In the microscopic RD model, the diffusion-limited regime can only be obtained after a sufficient number of particles has distributed along the Si-SiO<sub>2</sub> interface to form a common diffusion front.

### B. Limits of the Physical Validity of Rate Equations

In our calculations on the H-based RD model a new degradation regime emerges that is dominated by the equilibration between dangling bonds and the buildup of a diffusion front. This regime *cannot* be reproduced in a rate-equation based simulation even when more than one dimension and discrete dangling bonds are used, as shown in Fig. 4. Interestingly, the deterministic formulation always predicts a degradation curve that closely follows the one dimensional RD model rather than the stochastic version. This can be explained by the unphysical self-interaction in the reaction-rate based description, in which every hydrogen atom competes with itself for a dangling bond and the conversion into H<sub>2</sub> can even proceed from one single hydrogen atom. In contrast, in the microscopic stochastic model each hydrogen atom acts individually before the buildup of the diffusion front, which is certainly more physically reasonable. Therefore, only when each atom is considered separately, as in a stochastic simulator, the diffusion-front-buildup regime shows in the degradation curve. In deterministic solutions, the particles are *always* treated as a large ensemble, even in the regimes of very low concentrations, where this assumption is inappropriate.

### C. Modification of the Microscopic Model

It is interesting to note that the observation of the diffusion-limited regime after a certain degradation time in this simple

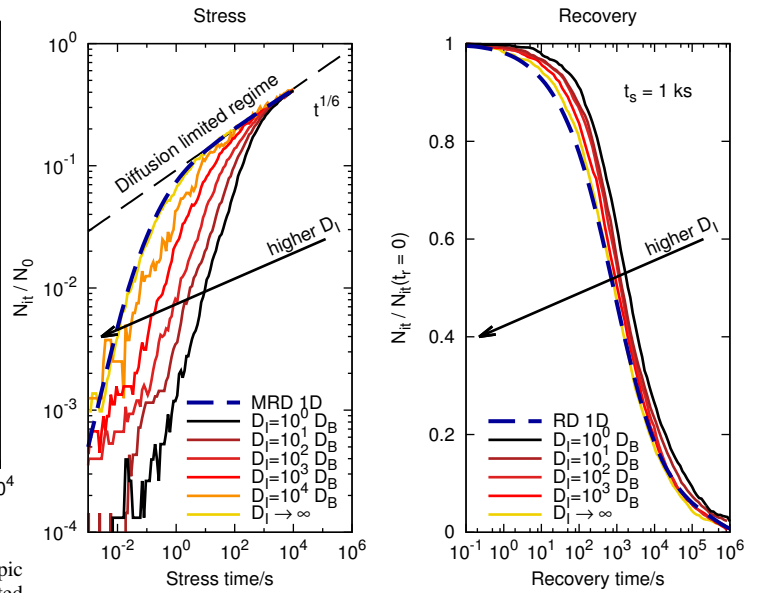


Fig. 5. Stress (left) and recovery (right) traces as predicted by our microscopic RD model and the influence of an increased interface diffusion coefficient  $D_I$ . **Degradation:** The increase of  $D_I$  reduces the lateral equilibration time. The newly observed diffusion front buildup regime becomes less pronounced in the degradation curve, leading to almost perfect agreement with the macroscopic model for  $D_I \rightarrow \infty$ . **Recovery:** Contrarily to the claims in [13], the recovery behavior of the three-dimensional stochastic RD model almost perfectly resembles the one-dimensional macroscopic recovery for all values of  $D_I$ . The deviation at low values of  $D_I$  comes from the lower degree of equilibration during stress time in these systems. As can be seen on the left side, after a stress time of  $10^3$  seconds, the systems with lower  $D_I$  have not yet fully entered the diffusion-limited regime.

formulation sets a lower boundary for the diffusion coefficient. This lower bound requires the diffusion front to extend several microns into the oxide or polysilicon gate in order to avoid saturation, which is certainly curious, considering the dimensions of modern gate stacks. There exists no comparable criterion for the macroscopic model.

To make the microscopic RD theory compatible with the macroscopic version, we consider first-principles calculations that have shown a lowering of diffusion barriers for hydrogen molecules along the Si/SiO<sub>2</sub> interface as compared to the bulk SiO<sub>2</sub> [25]. These findings indicate that the motion of hydrogen might proceed at a much higher rate along the interface, which aids the equilibration between the dangling bonds and therefore reduces the required bulk diffusion coefficient. To account for this in our microscopic model, we applied different diffusion coefficients  $D_I$  and  $D_B$  in the interface region and in the bulk, respectively [14].

### D. Stress and Recovery in the Microscopic Model

As can be seen in Fig. 5, the increase of the interface diffusion coefficient reduces the effect of lateral equilibration significantly. For a reasonable match between the microscopic and macroscopic RD model, an increase of four orders of magnitude is required, which corresponds to a diffusion coefficient of  $D_I \approx 1.6 \times 10^{-9}$  cm/s. While a diffusion coefficient of this magnitude may be hard to justify from a physical point-of-

view, it is still closer to the physical reality than the assumption of immediate equilibration along the Si-SiO<sub>2</sub> interface that is inherent to the usually employed one-dimensional macroscopic RD model. A perfect match between the microscopic and the macroscopic version of the RD model is only obtained in the limit  $D_1 \rightarrow \infty$ .

Interestingly, the three-dimensional stochastic motion of the hydrogen atoms and molecules *does not influence* the recovery behavior of the system, which contradicts the predictions of [13]. The recovery in the microscopic model matches the macroscopic version, which is incompatible with experimental data [5, 7, 8], independently of the choice of interface acceleration. This can be explained by the closed lateral boundary conditions in our calculations, which force the random motion of the diffusing hydrogen atoms into a straight path, therefore creating a laterally uniform distribution of particles which yields an effectively one-dimensional diffusive system during recovery. We have investigated the effect of open boundaries in [14] and found that the out flux of particles into the areas which are forbidden in closed boundary calculations again changes the degradation behavior, leading to an experimentally not observed and geometry dependent increase of the power-law slope during degradation. The closed boundary conditions on the other hand are equivalent to periodic boundary conditions and yield the behavior of an infinitely large Si-SiO<sub>2</sub> interface.

## V. CONCLUSION

We report on a stochastic three-dimensional implementation of the modified reaction-diffusion model for NBTI. The model is theoretically well-founded on the theory of stochastic chemical kinetics and is understood as a consequent realization of the physical picture behind the reaction-diffusion theory. It extends our previous efforts to microscopically simulate the hydrogen-atom-based RD model.

The degradation predicted by the microscopic model features a new regime which is dominated by the lateral equilibration of the diffusion cloud. This regime features a strongly increased power-law exponent and is not observed experimentally. It cannot be obtained from the usual macroscopic one-dimensional RD models, which *inherently assume* an *instant equilibration along the interface*. Further, it has been shown that the lateral equilibration regime cannot be properly modeled in *any* reaction rate based calculation, as in this description the many-particle interaction effects happen already at times where realistically the hydrogen atoms are still well separated.

The effect can only be reduced in a physically meaningful way by a strong increase of the diffusion coefficient along the interface. Perfect agreement between the microscopic and the macroscopic one-dimensional RD model is achieved in the limit  $D_1 \rightarrow \infty$ , which is the assumption that is inherent to all one-dimensional RD models.

Recent claims that a stochastic three dimensional description of the atomic diffusion could explain the long relaxation

tails observed in NBTI experiments while leaving the degradation untouched have been disproved by our calculations. The shape of the recovery arising from the reaction-diffusion theory is shown to be independent of the dimensionality and atomistic occupation effects by our calculations. Moreover, the microscopic description itself questions the physical relevance of the usually employed RD model. Especially its implicit assumption on the lateral equilibration in the early stages of degradation is difficult to justify.

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