Modeling of Dispersive Transport in the Context of Negative Bias Temperature Instability

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 Abstract—Negative bias temperature instability (NBTI) is one of the most serious reliability concerns for highly scaled pMOSFETs. It is most commonly interpreted by some form of reaction-diffusion (RD) model, which assumes that some hydrogen species is released from previously passivated interface defects, which then diffuse into the oxide. It has been argued, however, that hydrogen motion in the oxide is trap-controlled, resulting in dispersive transport behavior. This effect-controlled transport modifies the characteristic exponent in the power-law that describes the threshold-voltage shift. However, previous published models are contradictory and both an increase and a decrease in the power-law exponent have been reported. We clarify this discrepancy by identifying the boundary condition which couples the transport equations to the electro-chemical reaction at the interface as the crucial component of the physically-based description.

I. INTRODUCTION

Amongst the various reliability issues in modern CMOS technology, negative bias temperature instability (NBTI) has been identified as one of the most serious concerns for highly scaled pMOSFETs [1–4]. Recently, a lot of effort has been put into refining the classic reaction-diffusion theory [2, 5, 6] originally proposed by Jeppson and Svensson nearly thirty years ago [7, 8]. The RD model assumes that Si–H bonds at the interface are broken at higher temperatures and electric fields, causing the released hydrogen species to diffuse into the oxide. Analytic solutions of the RD model can be shown to follow a power-law [2]

\[
\Delta V_{th}(t) \propto \Delta N_{r}(t) = A(T, E_{ox}) t^n ,
\]

where the change in the threshold voltage is often assumed to be proportional to the change in the silicon dangling bond density \(N_{r} = [Si^*] \) at the interface. As diffusing species \(H_2\) is often assumed because in the RD framework it results in a characteristic time exponent of 1/6 for the threshold shift, consistent with recent no-delay measurements [9], while \(H^0\) and \(H^+\) result in \(n = 1/4\) and \(n = 1/2\), respectively [5].

During the last couple of years a variety of alternative explanations for NBTI have been put forward [3, 10–13]. In particular it has been argued that transport of the hydrogen species inside the oxide is dispersive [2, 10–12], consistent with hydrogen diffusion measurements and available models for irradiation damage. Interestingly, in these models the slope depends on a temperature-dependent dispersion parameter. Also, it is possible to incorporate technology-dependent behavior into the model by adjusting the dispersion parameter. In addition, these models brought \(H^+\) back into the game, which had originally been dismissed due to the 1/2 slope resulting from the RD model.

One feature common to trap-controlled dispersive NBTI models is that they predict that dispersive diffusion reduces the slope compared to their conventional counterparts [10–12]. However, in contrast to that it was observed that inclusion of traps into a standard RD model increases the slope [5]. In addition, our own simulations showed [14] that a straight-forward application of the multiple-trapping transport model [15, 16], which is the basis for many dispersive transport models [17], increases the slope, also in contradiction to published reaction-dispersive-diffusion models [2, 10–12]. A detailed analysis reveals that the boundary condition at the Si/SiO2 interface is the main reason for this discrepancy. It is shown that the choice of the boundary condition is essential for the overall behavior of the dispersive system.

II. DISPERSIVE TRANSPORT

In contrast to drift-diffusion transport, dispersive transport is trap-controlled. This implies that most particles are trapped, that is, bonded. Depending on the bonding energy (the distance to the ‘conduction band’) hydrogen can be easily released from shallow traps. With time, the demarcation energy becomes more negative, until the bottom of the trap distribution is reached and equilibrium is obtained. As a result, the motion of the particle packet slows down with time. Note how the individual trap levels, which microscopically correspond to the different bonding energies of hydrogen in an amorphous material, are approximated by a macroscopic density-of-states.

Fig. 1. Schematic illustration of dispersive transport. Particles in the conduction band fall into the traps and are re-emitted into the conduction band. Re-emission is more likely for shallow traps. The time-dependent demarcation energy separates shallow from deep traps. With time, the demarcation energy becomes more negative, until the bottom of the trap distribution is reached and equilibrium is obtained. As a result, the motion of the particle packet slows down with time. Note how the individual trap levels, which microscopically correspond to the different bonding energies of hydrogen in an amorphous material, are approximated by a macroscopic density-of-states.
that in the dispersive case most particles are trapped, that is, bonded, rather than in the ‘conduction state’. As will be shown, this issue is of fundamental importance to the model as it results in completely different time slopes.

A. Multiple-Trapping Model

Dispersive transport is often described using the continuous time random walk (CTRW) theory [19] or multiple-trapping (MT) models [15–17]. Both models exhibit similar features [20–22] and will be considered equivalent in the following [21]. The MT model equations consist of a continuity equation and the corresponding flux relation

\[
\frac{\partial H_c}{\partial t} = -\nabla \cdot f_c - \int \frac{\partial \rho}{\partial t} A E_t, \quad (2)
\]

\[
f_c = -D_c \left( \nabla H_c - \frac{Z}{V_T H_c E} \right). \quad (3)
\]

Here, \( H_c \) is the hydrogen concentration in the conduction state, \( D_c \) the diffusivity in the conduction state, \( Z \) the charge state of the particle, \( V_T \) the thermal voltage, \( E \) the electric field, while \( \rho(E_t) \) and \( g(E_t) \) are the trapped hydrogen density (cm\(^{-3}\)eV\(^{-1}\)) and density-of-states (cm\(^{-3}\)eV\(^{-1}\)) at the trap level \( E_t \). The trap occupancy is governed by balance equations which have to be solved for each trap level

\[
\frac{\partial \rho(E_t)}{\partial t} = \frac{\nu_0}{N_c} (g(E_t) - \rho(E_t)) H_c \quad \text{capture} \quad (4)
\]

\[
- \nu_0 \exp\left(-\frac{E_c - E_t}{k_B T_L}\right) \rho(E_t), \quad \text{release} \quad (5)
\]

with \( \nu_0 \) being the attempt frequency, \( N_c \) the effective density-of-states in the conduction band, \( T_L \) the lattice temperature, and \( E_c \) the conduction band edge (assumed to be zero in the following). In our context it is worthwhile to recall that the total hydrogen concentration consists of hydrogen in the conduction states \( H_c(x, t) \) and trapped hydrogen as

\[
H(x, t) = H_c(x, t) + \int \rho(x, E_t, t) dE_t \quad (6)
\]

An exponential density-of-states is commonly assumed [12, 17]

\[
g(E_t) = \frac{N_t}{E_0} \exp\left(-\frac{E_c - E_t}{E_0}\right), \quad (7)
\]

which, in this particular context, results in a power-law for \( N_t(t) \).

Qualitatively, the system responds as follows if brought out of equilibrium:

- At the initial stage, the capture rate (first term in (5)) dominates. Since \( \rho \) will still be small, the distribution will closely resemble the density-of-states (cf. Fig. 3).
- Then, since the release term depends exponentially on the distance of the trap level from the conduction band, particles on shallower traps (traps ‘closer’ to \( E_c \)) are more likely to be released than deeper traps. As a consequence, the shallower trap levels become depleted while particles accumulate in the ‘deep’ traps. This is the non-equilibrium regime.
- The transition between ‘shallow’ and ‘deep’ traps is described by the demarcation energy

\[
E_d(t) = E_c - k_B T_L \log \nu_0 t, \quad (8)
\]

which becomes more negative with time.

- As soon as the demarcation energy reaches the ‘bottom’ of the density-of-states, equilibrium is obtained, and the system behaves similarly to a non-dispersive one, although a different ‘effective’ diffusivity and temperature dependence are observed. Note, that from a mathematical point of view, this never happens for an ideal exponential density-of-states such as (7) [17].
The evolution of an initial particle sheet with time is shown in Fig. 2 while the trapped hydrogen profile \( \rho(E_t, t) \) is depicted in Fig. 3.

B. Extremely Non-Equilibrium Approximation

As the MT equations are rather complex and can in general only be solved numerically, simplified equations have been derived \[17\], valid in the extremely non-equilibrium case (EN-MT model). The approximation relies on the existence of the demarcation energy separating shallow from deep traps. The shallow traps are assumed to be in equilibrium with the conducting states while the deep traps create the dispersion due to the time dependent demarcation energy. Ignoring the initial early times and the possible final equilibration, one can show that the broadening of an initial particle distribution \( H_0(x) \) is given through

\[
H(x, t) - H_0(x) = -\nabla \cdot F(x, t) .
\]

(9)

Here the flux is given through an ‘effective’ flux of the total concentration of the species

\[
F = -D_c \left( \nabla H - \frac{Z}{V_F} \tau(t) H E \right) ,
\]

(10)

rather than the concentration in the conduction states \( H_c \). Note also, that there is no time derivative in (9) and the dynamics of the system can be incorporated into \( \tau(t) \), which directly depends on the hydrogen trap density-of-states

\[
\tau(t) = \left[ \frac{\nu_0}{N_c} \int_{E_t(t)}^{\infty} g(E_i) \, dE_i \right]^{-1} .
\]

(11)

Of particular interest in our context is the concentration of the ‘free’ hydrogen \( H_c \), which is directly linked to the total hydrogen concentration \( H \) and can be approximated in the non-equilibrium regime as \[17\]

\[
H_c(x, t) = \frac{\partial \tau(t) H(x, t)}{\partial t} .
\]

(12)

It is important to recall in our context that (9) was derived to describe the broadening of an initial particle distribution \( H_0 \), such as in Fig. 2. However, things are different during NBT stress where we have to deal with a continuous injection of particles into the oxide during the stress phase. A generalization of the original derivation reveals that (9) is still valid, provided the boundary condition is modified according to

\[
f_c(t) = \int_0^t f_c(t') \, dt' ,
\]

(13)

with \( f_c(t) \) being the particle influx at time \( t \). Note that (13) is only valid in the extremely non-equilibrium case which will be assumed to be prevalent in the following. The boundary condition (13) will be used for the numerical evaluation of (9).

III. DISPERVIVE TRANSPORT AND NBTI

In order to obtain an NBTI model, the transport equation has to be coupled to the electro-chemical reaction assumed to take place at the interface. As in the RD model \[8, 23, 24\], the kinetic equation describing the interface reaction is assumed to be of the form

\[
\frac{\partial N_{it}}{\partial t} = k_i (N_0 - N_{it}) - k_t N_{it} H_{it}^{1/\alpha} .
\]

(14)

where \( N_{it} \) is the surface state concentration, \( N_0 \) the initial concentration of passivated interface defects, \( H_{it} \) the interfacial hydrogen concentration, \( k_i \) and \( k_t \) the field and temperature dependent rate coefficients, while \( \alpha \) is the kinetic exponent (1 for \( H^0 \) and \( H^+ \), and 2 for \( H_2 \) \[24\]).

As a boundary condition to the transport equations one has

\[
f_c(t) \cdot n = \frac{1}{a} \frac{\partial N_{it}}{\partial t} ,
\]

(15)

with \( n \) being the normal vector at the interface. For the non-equilibrium approximation we obtain through (13)

\[
F_c(t) \cdot n = \frac{N_{it}(t) - N_{it}(0)}{a} .
\]

(16)

Classic and dispersive NBTI models assume the interface reaction to be in quasi-equilibrium \( (\partial N_{it}/\partial t \approx 0) \) \[2, 10, 12\]. From (14) one obtains by neglecting saturation effects \( (N_{it} \ll N_0) \)

\[
\frac{k_t N_0}{k_i} = N_{it} H_{it}^{1/\alpha} .
\]

(17)

A. Total Hydrogen Boundary Condition

The fundamental question in the context of dispersive transport is how to determine the interfacial hydrogen concentration \( H_{it} \). In \[12\] it was assumed that the NBTI reverse reaction is driven by the total hydrogen concentration at the interface, that is \( H_{it}(t) = H(0, t) \).

Equation (9) is straightforward to solve and assuming the interface at \( x = 0 \), the total hydrogen concentration in the positive half-space is given as

\[
H(x, t) = H(0, t) \exp \left( -\frac{x}{\lambda(t)} \right) ,
\]

(18)

with \( \lambda(t) = \sqrt{D_c \tau(t)} \) for neutral particles and \( \lambda(t) = \mu_c E_{ox} \tau(t) \) for protons \[12\], with \( \mu_c = q D_c / k_B T_L \).

Integrating (9) over the half-space \( x > 0 \) we obtain with (16) and (18) together with \( N_{it}(0) = 0 \) and \( H_0(x, 0) = 0 \)

\[
N_{it}(t) = \alpha \lambda(t) H(0, t) .
\]

(19)

Assuming \( H_{it}(t) = H(0, t) \) and plugging (19) into (17) we obtain for neutral particles \( (Z = 0) \)

\[
N_{it}(t) = A \left( \frac{N_0}{N_{it}} \right)^{1/(2+2a)} \left( \nu_0 t \right)^{\alpha/(2+2a)} ,
\]

(20)

with the dispersion parameter

\[
\alpha = k_B T_L / E_0 .
\]

(21)

The prefactor \( A \) is given through

\[
A = \left( k_t N_0 / k_i \right)^{\alpha/(1+\alpha)} (\alpha^2 D / \nu_0)^{1/(2+2a)} .
\]

(22)

For atomic hydrogen \( (\alpha = 1) \) the slope is given through \( n = \alpha/4 \) while molecular hydrogen \( (\alpha = 2) \) gives \( n = \alpha/6 \). Since \( \alpha \) equals 1 in the diffusive limit and 0 in the extremely dispersive case, (20) implies that for dispersive transport a slope smaller than the RD slopes of 1/4 and 1/6 can be obtained. Also, for increasing trap density \( N_c \), the total amount of degradation decreases. With \( Z = 1 \) and the approximate relation for \( \lambda(t) \) we obtain \( n = \alpha/2 \) for \( H_+ \). Note that the numerical solution for \( H_+ \) contains a transitional region with \( n = \alpha/4 \), where the diffusive component still dominates.

Qualitatively, this means that dispersive transport results in most particles being trapped close to the interface, resulting in a steeper profile compared to classic diffusion. However, as all hydrogen is available for the reverse rate in (14), the net interface state generation is suppressed, resulting in a smaller slope.

Since the dispersion parameter \( \alpha \) depends linearly on the temperature, a linear temperature dependence of the slope is obtained as \[12\]

\[
n = \frac{\alpha}{2+2a} = \frac{k_B T_L}{2E_0 (1+a)} .
\]

(23)
This is consistent with experimental results [3, 12]. It has to be kept in mind, however, that these data were obtained using delayed measurements and also temperature-independent slopes for delay-free measurements have been reported [9].

**B. Conduction State Hydrogen Boundary Condition**

In contrast, if we now assume that only the free hydrogen can participate in the reverse rate, that is \( H_t = H_t(0) \), which is the 'natural' boundary condition for the MT model [25], one obtains

\[
\frac{k_t N_0}{k_i} = N_{H_t}(t) \left( \frac{\tau(t)}{a\lambda(t)} \frac{\partial}{\partial t} \right)^{1/\alpha},
\]

which for neutral particles (\( Z = 0 \)) has the solution

\[
N_{H_t}(t) = A \left( \frac{N_0}{N_c} \right)^{1/(2+2\alpha)} \left( \frac{1 + a}{1 + a/2} \right)^{(1+\alpha)/(1+\alpha/2)} \left( \frac{\nu t}{a\lambda^\alpha} \right)^{(1-\alpha/2)/(1+\alpha)}.\]

For atomic hydrogen, the slope \( n = 1/2 - \alpha/4 \) is obtained while \( H_2 \) results in \( n = 1/3 - \alpha/6 \). Hence, for increased dispersion the slopes become now larger than their RD equivalents. Furthermore, when the trap density is increased, the degradation increases. In contrast, \( H^+ \) results in \( n = 1/2 \), which is equal to the classic result and independent of the dispersion parameter!

Again, qualitatively, the newly released hydrogen quickly falls into the traps (becomes bonded again), but since for times larger than \( 1/\nu_0 \) most hydrogen resides in deep traps and is therefore not as easily available for the reverse rate in (14). This suppresses the reverse reaction and consequently enhances the net interface state generation and results in a larger slope.

In contrast to the previous boundary condition, now the slope decreases with increasing temperature through

\[
n_2 = \frac{1 - \alpha/2}{1 + a} = \frac{2E_0 - k_B T_1}{2E_0 (1 + a)} = \frac{1}{1 + a} - n_1.
\]

This is in contradiction to currently available observations [3, 9, 12].

The possible slopes for the various combinations of boundary condition and species are compared in Fig. 4.

**C. Alternative Models**

Instead of the MT model, an approximate solution for the CTRW models was employed by Houssa et al. [11]. Again, this approximate solution was derived for the broadening of an initial concentration [26], and since CTRW and MT theory are in many ways compatible [20, 21], we assume our results of the MT model to also apply to models derived from the CTRW theory.

Instead of MT or CTRW solutions, models based on a phenomenological time-dependent diffusivity

\[
D(t) = D_0 (\nu t)^{-(1-\alpha)},
\]

have been used [2, 10]. Here, \( D_0 \) is the microscopic diffusivity, \( \nu \) an attempt frequency different to \( \nu_0 \), and \( \alpha \) the dispersion parameter [27]. As in the MT model for an exponentially decreasing trap density, \( \alpha \) is given as \( \alpha = k_B T_1/E_0 \), where \( E_0 \) is the characteristic energy. Since (27) is derived by matching SIMS measurements, this model does not allow one to differentiate between free and trapped hydrogen, which has a significant influence on the NBTI boundary condition as shown below.

**IV. MODEL COMPARISON**

A numerical solution of the MT model was used as a reference model. For the numerical solution the trap density-of-states was discretized using 20 energy points while the energy range was limited to the interval \( E_{max} = 0 \text{ eV} \) and \( E_{min} = -20E_0 \). This implies that as soon as the demarcation energy \( E_d \) reaches \( E_{min} \), a transition from the dispersive to the classic diffusive regime is observed. Note that this transition is not available in the approximate solutions described above. As the exact value of \( E_{min} \) is essentially unknown, it was set to a value small enough so as not to influence the numerical solution. Furthermore, the numerical solution considers the trap occupancy in the capture rate of (5), which is also not contained in the approximate solutions. This trap occupancy results in a transition from dispersive to conventional diffusion as soon as all traps are filled. Such a transition might be relevant and can also be experimentally observed for hydrogen concentrations larger than

![Graph showing interface state density as a function of the boundary condition](image-url)
the trap density \([18]\). However, this effect is neglected here for the sake of a straight-forward comparison.

In a first step the applicability of the Arkhipov model to NBTI is investigated. For this the numerical solutions of the MT and the EN-MT equations are compared in Fig. 5 where good agreement is observed for each boundary condition, thereby justifying the underlying approximations. Next, the analytical expressions (20) and (25) are compared to the numerical solutions of the MT equations in Fig. 6. Again, good agreement is obtained in the quasi-equilibrium (diffusion-limited) regime. Of course, no reaction-limited regime and the continuous injection of particles is too slow \((\partial N_\text{t}/\partial t \approx 0)\) to seriously disrupt the extremely non-equilibrium assumption with a single demarcation energy.

The amount of hydrogen that is allowed to participate in the reverse reaction determines the overall dynamics, that is, this boundary condition determines whether an increase or a decrease in the slope is observed.

The temperature dependence of the slopes predicted by the analytic expressions (20) and (25) are compared to the full numerical results in Fig. 8. Note that the system is only dispersive as long as the characteristic energy \(E_\text{0}\) in the density-of-states \((7)\) is larger than the thermal energy \(k_B T\) \([17]\). In terms of the dispersion parameter \(\alpha\) this means \(\alpha < 1\). This also implies that for increasing temperatures a transition to classic transport is observed as soon as \(E_\text{0}\) becomes smaller than the thermal energy \(k_B T\), that is, \(\alpha > 1\). Since the dispersive models are derived under the assumption \(\alpha < 1\), the cannot reproduce the full numerical results in that regime, but give excellent agreement for \(\alpha < 1\).

The good agreement between the numerical and analytic result indicates that the simplifying assumptions in the derivation of (20) and (25) are well justified, which are worth summarizing:

- The dynamics are solely determined by carrier trapping and detrapping.
- The continuous injection of particles is too slow \((\partial N_\text{t}/\partial t \approx 0)\) to seriously disrupt the extremely non-equilibrium assumption with a single demarcation energy.
- The amount of hydrogen that is allowed to participate in the NBTI reverse reaction determines the overall dynamics, that is, this boundary condition determines whether an increase or a decrease in the slope is observed.
- The interface reaction is in quasi-equilibrium.

V. CONCLUSIONS

Clearly, the question of what boundary condition for the reverse rate in the NBTI model captures the microscopic physics best is of utmost importance. For the present analysis we have to keep in mind that the macroscopic density-of-states is derived for a amorphous bulk material and is unlikely to be valid next to an interface. In that context, the physical mechanisms justifying the 'conduction band' concept in conjunction with hydrogen hopping next to the interface need to be evaluated and justified.

Under the assumption that this concept remains nevertheless valid, we have investigated two different boundary conditions: Provided
that only hydrogen in the multiple-trapping conduction band can passivate dangling bonds, only H$_2$ in a reaction-dispersive-diffusion model gives slopes compatible with measurements and would allow to explain (temperature-dependent) delay-free slopes larger than 1/6. In contrast, if all the trapped hydrogen can be involved, the previously published NBTI models [2, 10–12] remain valid, reproducing (temperature-dependent) measured slopes also with H$^0$ and H$^+$ kinetics.

REFERENCES


