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1 Electromigration Modeling for Interconnect Structures in Microelectronics

Electromigration is one of the most important reliability issues in semiconductor technology. Its complex character demands comprehensive physical modeling as basis for analysis. Simulation of electromigration induced interconnect failure focuses on the life-cycle of intrinsic voids, which consists of two distinct phases: void nucleation and void evolution. We present models for both phases as well as models which describe the impact of metal microstructure and mechanical stresses. These stresses have their sources in the fabrication process itself and in the material transport caused by electromigration. Special emphasis is put on explaining the void morphology and its impact on interconnect resistance. Investigations for common two- and threedimensional interconnect structures are presented. Implications of the theoretical analysis and the simulation results for modern interconnect design are discussed.

1.1 Introduction

Failure of metallic interconnects in integrated circuits caused by electromigration has long been a key reliability concern which is further accentuated by the continuing trend of miniaturization. The phenomenon of electromigration is a mechanism for transport of matter by high electric current densities which produce damage in the interconnect lines. Failure results either from voids growing over the entire line width or extrusions which cause short circuits to neighboring lines.

Copper with its lower resistivity, higher melting point, good mechanical strength, and better electromigration performance [1, 2] has replaced aluminum as advanced metalization solution. However copper based interconnects have introduced new problems, since copper electromigrates along fast diffusion paths at the interfaces to surrounding layers [3, 4].

The main challenge in electromigration modeling and simulation is the diversity of the relevant physical phenomena. Electromigration induced material transport is also accompanied by material transport driven by the gradients of material concentration, mechanical stress, and temperature. A comprehensive, physics based analysis of electromigration for modern copper interconnect lines serves as basis for deriving sophisticated design rules which will ensure higher steadfastness of interconnects against electromigration.

The material transport driven by electromigration is most commonly modeled by the dynamics of crystal vacancies. A high concentration of vacancies or high tensile stress indicates sites where the nucleation of intrinsic voids is very probable. The main task of electromigration modeling and simulation is a prediction of the hot spots in the interconnect geometry where stress and vacancy concentration reach their peak values as well as the time needed for these values to be reached assuming usual operating conditions.

1.2 Electromigration Failure Mechanism

The development of intrinsic voids, which leads to interconnect failure, goes through two distinctive phases. These phases exhibit the different influence on the operating abilities of interconnects and are based on different physical phenomena.

The first phase is the void nucleating phase in which electromigration-generated voids do not exist and a significant resistance change is not observable. The second phase starts when a void is nucleated and becomes visible in SEM pictures [5].

This is the so-called rapid phase of void development. The void expands from its initial position (nucleation site) to a size which can significantly change the resistance or completely sever the connection. If we denote the void nucleation time with t_N and the void evolution time with t_E , the time to failure t_F is,

$$t_F = t_N + t_E. \tag{1}$$

The expected resistance development during these time periods is sketched in Fig. 1. The development of a general electromigration model demands a careful analysis of physical phenomena in both phases of void development.

1.3 Void Nucleation

The electromigration model applied in this work is based on propositions made in [6]. The model connects the



Figure 1: Resistance behavior and failure development phases.

1 Electromigration Modeling for Interconnect Structures in Microelectronics

evolution of the mechanical stress with the diffusion of vacancies under full account of the influence of the geometry of the metalization.

The dynamics of the vacancies is described by the following two equations [6,7]

$$\mathbf{J}_{\nu} = -D_{\nu} \left(\frac{Z^* e}{k_B T} C_{\nu} \nabla \boldsymbol{\varphi} + \nabla C_{\nu} + \frac{f \Omega}{3 k_B T} C_{\nu} \nabla \operatorname{tr}(\boldsymbol{\sigma}) \right), \quad (2)$$
$$\frac{\partial C_{\nu}}{\partial t} = -\nabla \mathbf{J}_{\nu} + G(C_{\nu}), \quad (3)$$

where C_v is the vacancy concentration, f is the vacancy relaxation ratio, Ω is the atomic volume, D_v is the vacancy diffusivity, k_B is Boltzmann's constant, T is the local temperature, Z^*e is the effective valence, and $G(C_v)$ is the source function which models vacancy generation and annihilation processes. A closer look at equation (2) reveals that three major driving forces induce the dynamics of vacancies: the electromigration which is proportional to $\nabla \varphi$, the concentration gradient, and the mechanical stress gradient $\nabla \operatorname{tr}(\sigma)$.

If there is no residual mechanical stress from the technological process flow and an initially uniform distribution of vacancies (as is normally the case), it is obvious that the rise of mechanical stress and concentration gradients is a response to the electromigration stressing of the interconnect material. The overall behavior of temperature gradients depends on the material choice, the geometry of the interconnect layout, and the operating conditions. Both scenarios, in which temperature gradients enhance or retard vacancy transport induced by electromigration, are possible.

Considering the effective vacancy diffusivity we can distinguish between three basic diffusion paths and their diffusivities: bulk, grain boundaries, and copper interfaces to other layers. Interface self-diffusion is the dominant diffusion mechanism for the case of standard barrier layers such as TiN, as shown by many experimental observations [8,9].

In his pioneering work on electromigration Korhonen *et al.* [10] use a direct relationship between lattice density and hydrostatic stress. This approach is based on simplifications which are justifiable only for a straight aluminum line. Other researchers, such as Povirk [11] and Rzepka *et al.* [12], searched for a more general description and employed the idea that diffusion fluxes give rise to volumetric strain which serves to establish stress fields, thereby driving stress-migration fluxes.

Using a similar concept, Sarychev and Zhitnikov [6] introduced a contribution of local vacancy dynamics to stress build-up in a three-dimensional model of stress evolution during electromigration. The standard elastic model was extended by introducing inelastic loads due to vacancy migration and recombination. The total strain tensor is given by

$$\varepsilon_{ik} = \varepsilon_{ik}^{\nu} + \varepsilon_{ik}^{\sigma}, \qquad (4)$$

where ε_{ik}^{ν} and $\varepsilon_{ik}^{\sigma}$ denote the inelastic and elastic strain component, respectively. The kinetic relation for inelastic strain component is given by [13],

$$\frac{\partial \varepsilon_{ij}^{\nu}}{\partial t} = \Omega \Big[(1-f) \nabla \mathbf{J}_{\nu} + f \frac{C_{\nu} - C_{\nu}^{eq}}{\tau} \Big] \delta_{ij}.$$
(5)

During the material redistribution induced by any driving force, the lattice actually tries to keep the vacancy concentration at its equilibrium value.

An even more complete model than this presented above also includes diffusion in the grain boundaries together with an interaction model which describes the vacancy exchange between the grain boundaries and the bulk. A model of this type was first studied by Fisher [14] and represents a promising improvement for electromigration modeling.

The lack of well-established models for nucleation of initial voids remains a limitation in modeling the failure of interconnect lines. Typically used nucleation conditions are critical stress or/and critical vacancy concentration [15], but in both cases it is actually very difficult to motivate values of these thresholds.

Consideration based on classical thermodynamics and kinetics [16] have shown that for aluminum, the nucleation rates for bulk, grain boundary, and sidewalls are very low. Such an analysis has, to the authors knowledge, not been carried out for copper technology.

1.4 Void Evolution

Modeling the micromechanics of void evolution is a long-standing scientific problem. It began with sharp interface models requiring an explicit finite element tracking of void surfaces during the course of evolution [17]. Later, prompted by the complexity of void surfaces, diffuse interface (DI) models were introduced [18–20].

Diffuse interface models circumvent computationally costly explicit surface tracking by application of a smooth order parameter field for the representation of void structures. An alternative diffuse interface model based on the double obstacle potential was proposed in [21], where the computation is simplified by reduction of order parameter profile evaluation to only the void-metal interfacial area.

The main disadvantages of these diffuse interface models are their requirement of underlying structured meshes for the order parameter evaluation and their restricted capability to reach higher resolution of an order parameter profile in the void-metal interfacial area.

In the case of void evolution there are two main forces which influence the shape of the evolving void interface: the chemical potential gradient and the electron wind. The first force causes self-diffusion of metal atoms on the void interface and tends to minimize energy, which results in circular void shapes. The electron wind force produces asymmetry in the void shape depending on the electrical field gradients.

Including both contributions, electromigration and chemical potential-driven surface diffusion, gives the total surface vacancy flux, $J_s = J_s t$, where t is the unit vector tangent to the void surface [17, 22]

$$J_{s} = -D_{s}\left(eZ^{*}E_{s} + \Omega\nabla_{s}\left(\frac{\sigma:\varepsilon}{2} - \gamma_{s}\kappa\right)\right).$$
(6)

 $E_s \equiv \mathbf{E_s} \cdot \mathbf{t}$ is the local component of the electric field tangential to the void surface, ∇_s is the surface gradient operator, $0.5 (\sigma : \varepsilon)$ is the strain energy density of the material adjacent to the void surface, and κ is the curvature of the void surface. D_s is given by an Arrhenius' law:

$$D_s = \frac{D_0 \,\delta_s}{k_B T} \exp\left(-\frac{Q_s}{k_B T}\right). \tag{7}$$

Here, δ_s is the thickness of the diffusion layer, Q_s is the activation energy for the surface diffusion, and D_0 is the pre-exponential coefficient for mass diffusion. Equation (6) is the Nernst-Einstein equation, where the sum in the parentheses on the right side expresses the driving force. Mass conservation gives the void propagation velocity normal to the void surface, v_n , through the continuity equation,

$$v_n = -\nabla_s \mathbf{J_s}.$$
 (8)

The full simulation scheme including void nucleation and void evolution is presented in Fig. 2.

The simulation loops in the both phases (Fig. 2) are needed for a prediction of the time to failure of the interconnect (1). The simulation in the second phase also determines resistance fluctuations.

1.5 Surface Tracking by Diffuse Interface Models

Direct numerical implementation of equations (6)-(8) demands explicit tracking of the moving void-metal interface. The interface is described by specifying a large number of points on it. Over the time the void-metal interface evolves and changes morphology and even more points may be required to accurately describe it. Such techniques are very complicated to implement and also tend to have rather poor numerical stability.

In the diffuse interface models void and metal area are presented through the order parameter ϕ which takes values +1 in the metal area, -1 in the void area and $-1 < \phi < +1$ in the void-metal interface area. Demanding explicit tracking of the void-metal interface is not needed and models do not require boundary conditions to be enforced at the moving boundary. Diffuse interface models are, as we will see in the next sections, quite simple to implement numerically.

The model equations for the void evolving in an unpassivated interconnect line are the balance equation for the



Figure 2: Two-phase electromigration simulation scheme.



Figure 3: Current density distribution and applied finite element mesh.



Figure 5: Electromigration induced vacancy distribution.

order parameter ϕ [18, 21],

$$\frac{\partial \phi}{\partial t} = \frac{2D_s}{\varepsilon \pi} \nabla \cdot (\nabla \mu - |e| Z^* \nabla V) \tag{9}$$

$$\mu = \frac{4\Omega\gamma_s}{\epsilon\pi} (f'(\phi) - \epsilon^2 \Delta\phi) \tag{10}$$

and for the electrical field

$$\nabla \cdot (\sigma(\phi) \nabla V) = 0 \tag{11}$$

where μ is the chemical potential, $f(\phi)$ is the double obstacle potential as defined in [23], and ε is a parameter controlling the void-metal interface width. The electrical conductivity was taken to vary linearly from the metal ($\sigma = \sigma_{metal}$) to the void area ($\sigma = 0$) by setting $\sigma = \sigma_{metal}(1 + \phi)/2$.

1.6 Simulation Results

In order to illustrate capabilities and consequences of the introduced models we consider two examples. The vacancy dynamics leading to void nucleation is studied for the case of a dual-damascene architecture consisting of copper, capping, and diffusion barrier layers, and void



Figure 4: Temperature distribution.



Figure 6: Interconnect via with initial void.

evolution for the case of a void nucleated in the bulk of the interconnect (Fig. 6).

The structure was generated applying a typical damascene process flow using DEP3D [24] for the deposition of the TiN barrier layer, copper, and dielectric (silicondioxide). For the emulation of the other deposition, etching, and polishing process steps, DEVISE [25] was used.

During the operation of the interconnect a redistribution of vacancies under the influence of the various promoting factors takes place. The increase of the vacancy concentration, i.e. depletion of material at specific places in the interconnect metal, leads to build-up of tensile stress. The simulated current density distribution together with the finite element mesh used is presented in Fig. 3 and the temperature distribution in Fig. 4.

Starting from uniformly distributed vacancies, during the operation of the interconnect local peaks of the vacancy concentration can be observed (Fig. 5). If a balance between electromigration, vacancy concentration, temperature, and mechanical stress gradients, which characterizes the operating condition of the interconnect, is reached, the vacancy concentration will remain at some value independent of time: the interconnect structure is virtually immortal. The interconnect layout and operating conditions chosen in the presented example produce a situation where the vacancy concentration remains stable at 6.5×10^{15} cm⁻³. This concentration is well below the lattice sites concentration of 10^{23} cm⁻³, but it still represents a supersaturation of approximately 3000 times the equilibrium value for 300° C.

As a setting for a void evolution example we consider a two-dimensional, stress free, electrically conducting interconnect via. A constant voltage is applied between points A and B (Fig. 6). At B a refractory layer is assumed. Because of geometrical reasons there is current crowding in the corners C and D. High electrical field



Figure 7: Void evolving through interconnect in the electric current direction

gradients in the area around the corners increase the overall error of the finite element scheme, which is overcome by applying an additional refinement of the finite element mesh according to the local value of the electric field. A fine triangulated belt area which is attached to the voidmetal interface [22] at the initial simulation steps follows the interfacial area throughout the simulations, whereby the interconnect area outside the interface is coarsened to the level of the initial mesh.

In our simulations a void evolving through the straight part of the interconnect geometry exhibits similar shape changes as observed in earlier models [17]. There is also no significant fluctuation of the resistance during this period of void evolution (Fig. 8). The situation changes,



Figure 8: Time dependent resistance change during void evolution for the different initial void radius *r*.

Figure 9: Mesh adaptation in the case of void collision with the refractory layer.

when the void evolves in the proximity of the interconnect corner. Due to current crowding in this area the influence of the electromigration force on the material transport on the void surface is more pronounced than the influence of the chemical potential gradient. This leads to higher asymmetry in the void shape then observed in the straight part of the interconnect. A void evolving in the proximity of the interconnect corner causes significant fluctuations in the interconnect resistance due to asymmetry and position. The resistance change shows a characteristic profile with two peaks and a valley (Fig. 8).

The extremes are more pronounced for larger initial voids. The capability of the applied adaptation scheme is also presented in the simulation of void collision with the interconnect refractory layer (Fig. 9).

Our simulations shows that for all considered initial void radii, voids follow the electric current direction (Fig. 9) and do not transform in slit or wedge like formations which have been found to be the main cause for complete interconnect failure [26].

The applied diffuse interface model extends readily to incorporate additional physical phenomena such as anisotropy, temperature variations, and bulk and grain boundary diffusion.

1.7 Conclusion

The electromigration reliability analysis of modern interconnects demands simulation tools which are based on comprehensive physical models. In order to predict an interconnect failure, modeling and analysis of complete life cycles of electromigration induced intrinsic voids are needed.

A careful analysis of the connection between the local vacancy dynamics and strain build-up must be carried out. The obtained relations have been coupled to an electromigration model using the concepts of stress driven diffusion and anisotropy of the diffusivity tensor. For correct physical handling of the grain boundary network as the network of high diffusivity paths and at the same time as sites of vacancy recombination, a method of splitting a copper segment into grain segments is introduced. The grain boundary segments are treated as simulation sub-domains connected to each other by diffusive, mechanical, and electrical interface conditions. A dualdamascene architecture example layout is used to illustrate and verify the introduced modeling approach. The obtained simulation results qualitatively resemble the behavior observed in experimental investigations.

A governing equation for the void evolution is solved using the finite element scheme. A dynamically adapted mesh is maintained by a refinement-coarsening algorithm controlled by position, curvature, and width of the simulated void-metal interface, which distributes the mesh density in such a way, that it allows efficient simulation of evolving voids through large portions of a complex interconnect geometry. Due to high electrical current gradients in the proximity of the interconnect corners and overall asymmetry of the electrical field, voids exhibit a specific faceting which was not observed in the case of straight interconnect geometries.

The presented method is well suited for long time prediction of resistance change due to electromigration during the interconnect life time. The applied diffuse interface model can be extended readily to incorporate additional physical phenomena such as anisotropy, temperature variations, and bulk and grain boundary diffusion.

2 An Energy-Level Perspective of Bias Temperature Instability

Many recent publications discussing the stress and recovery behavior of bias temperature instability (BTI) have suggested the existence of two components contributing to the phenomenon. One of these components was found to be quickly relaxing while the other was only slowly relaxing or even permanent. Curiously, although the most likely suggested mechanisms are the generation of interface states and the capture of holes into pre-existing traps, there is no agreement on which mechanism corresponds to which component and both possibilities have been suggested. Alternatively, other groups have suggested evidence that BTI is dominated by a single mechanism, and used the reaction-diffusion (RD) model to describe the degradation. However, RD theory cannot explain the recovery and related intricacies of the phenomenon.

We present a new modeling framework based on the various possible energetic configurations of the system and tentatively assign these levels to the hydrogen binding/transport levels in an amorphous oxide. We investigate the possibility that the often observed recoverable and permanent components are in fact two facets of a single degradation mechanism proceeding as a series of steps. We finally subject the model to various experimental data (DC, AC, duty-factor, negative and positive stress, mixed stresses) which are all well reproduced by the model.

2.1 Introduction

After four decades of research, bias temperature instability (BTI) is still a highly puzzling phenomenon which has so far eluded our complete understanding [27–30]. Particularly intriguing are the complex degradation/recovery patterns which are observed when the gate bias is modulated [31–34]. Understanding this behavior is mandatory for any estimation of device degradation in a circuit setting.

Quite contrary to these experimental observations, most modeling approaches published so far have focused on constant gate bias stress and are remarkably oblivious to any recovery of the degradation which sets in as soon as the stress is removed. This dilemma is easily illustrated using the reaction-diffusion (RD) model [35, 36] as the most prominent example: the RD model describes the stress phase as a delicate interplay between the reaction-limited forward rate and the diffusion-limited backward rate [37]. The forward rate alone would predict a degradation directly proportional to the stress time t_s , while only in combination with the backward rate the ominous $\sim t_s^{1/6}$ time-dependence is obtained. During recovery, the backward-rate can be studied on its own, predicting recovery to occur basically within four decades of time, in stark contrast to the experimentally observed log-like recovery over twelve decades [34, 38]. Recent attempts to rectify this problem [39–42] have so far been unsatisfactory [30].

Triggered by the interest in the origin of the recovery [31, 43], the last couple of years have seen a lively debate on whether NBTI is caused by interface states alone [29] or whether the observed degradation is a superposition of interface state generation and hole capture into pre-existing traps [27, 44–47]. In particular, charge-pumping (CP) experiments have delivered results which are quite different from degradation observed during electrical measurements. For instance, it has been observed that the CP signals show a remarkably different recovery behavior compared to conventional data. This and similar facts have been used to separate the overall degradation into interface state and hole trapping contributions.

In our recent studies [34, 38] we have demonstrated how the wealth of information present in the recovery data can be used to deepen our understanding of the phenomenon. Utilizing the universality of the recovery [38, 48] we have extracted a fast and universally recovering component which is observed on top of a permanent or very slowly recovering component.

The existence of two components appears to be consistent with a growing number of recent publications [27, 44–46]. The fast universally recovering component is often identified as hole trapping while the permanent or slowly recovering component may be caused by interface states. Curiously, however, contradictory explanations have also been given speculating that deep hole traps form the permanent component [44].

From a physical point of view these interpretations would mean that two independent degradation mechanisms act in parallel with only the overall degradation being visible. While an NBTI model may eventually be constructed using such two individual components [27,38], one may ask if these two components are in fact not parallel but act in series and are therefore two facets of a single degradation mechanism proceeding in steps. Such a view is supported by the fact that the degradation of the drain current (actually, $I_D(t_s) - I_D(1 \text{ ms})$) in a simple on-the-fly (OTF) measurement obtained at different temperatures and voltages can be made to overlap using simple scaling (see Figure 10 and Figure 11). If two independent mechanisms were to contribute to NBTI, it would be highly unlikely for these mechanisms to have a similar voltage and temperature acceleration, because only then would a superposition of these two mechanisms result in such a scalability. In fact, quite different



Figure 10: The change in the drain current recorded in an on-the-fly (OTF) measurement with an initial delay of 1 ms at different temperatures for an oxynitride PMOS with EOT = 1.4 nm. The OTF measurement is interrupted periodically to record 12s long relaxation sequences. Data obtained at the same stress voltage (-2V) can be made to overlap by multiplication with a suitably chosen (temperature-dependent) factor, given in the legend.

activation energies have been extracted for such two possible mechanisms [34] which appears to be inconsistent with the apparent scalability of the data. Also, PBTI and mixed negative/positive stresses (NBTI/PBTI), as shown in the following do not seem to be consistent with the hole-trapping model suggested by Tewksbury [49] and suggested for NBTI by Huard *et al.* [27], since independently of the stressing voltage, *positive* charge is created in the device (at least for the samples used in this study). However, creation of positively charged defects is consistent with donor-like (or amphoteric) states [50, 51] in the silicon bandgap [52] which are able to rapidly exchange charges with the silicon substrate and thus appear as positive charges when measured at $V_G = V_{th}$.

As previously suggested, we first direct our efforts at understanding the peculiarities of recovery [38]. A particularly noteworthy property of the recovery is its nearly logarithm-like character lasting at least twelve decades in time [34, 53]. This kind of recovery can be empirically described by various analytic expressions, including the stretched-exponential form [38], which is characteristic to an abundance of diverse physical phenomena (dielectric relaxation, voltage recovery in Leyden bottles, recovery of mechanical strain in wires, decay of luminescence in wires, etc. [54]) and commonly attributed to some kind of disorder. One modeling approach considers such systems as having two closely coupled energetic minima, the equilibrium and a slightly higher second minimum separated by an energy barrier [55, 56]. This barrier may either be surmounted by thermal excitation or by quantummechanical tunneling [56, 57]. During the application of stress, the second minimum may be lowered below the equilibrium minimum, making it the preferred energetic state. Depending on the transition mechanism and the statistical distribution of these barrier energies, a timedependent transition between the two wells is observed. Once the stress is removed, the equilibrium well will be occupied again, which commonly involves long recovery transients.

Based on these principles we will develop a new model for bias temperature instability in the following which provides an explanation for the issues raised in our previous work [30, 34, 38]. In particular, we do not just consider the stress phase for the formulation of our theory, but put equal emphasis on a correct description of the recovery phase [31]. Consequently, the model is evaluated for DC NBTI/PBTI stress and recovery, duty factor dependence, and mixed NBTI/PBTI stresses.

2.2 An Energy-Level Perspective

Our new model can be understood in terms of previously suggested mechanisms for the dissociation of siliconhydrogen bonds, which creates an electrically active defect, for instance a P_b center at the SiO₂/Si interface or a K_N center inside SiON [52]. In equilibrium, that is, after the passivation step used during fabrication and before application of stress, most hydrogen atoms are bound to silicon dangling bonds, which represents the ground state. Such a scenario is schematically sketched in Figure 12. However, this is not the case for all configurations as wells are assumed to exist where a site next to the dangling bond is energetically favored. This is a reasonable assumption because during passivation it is possible to passivate a large number of interface states (e.g. 10^{12} cm⁻²) but not all (e.g. 10^9 cm⁻² remain).

Upon application of an electric field and at elevated temperatures the hydrogen atom may overcome the barrier to the neighboring transport state via thermal emission [56]. Alternatively, particularly at low temperatures, the hydrogen may tunnel from an excited level to the transport state. Such a mechanism has been suggested for dielectric relaxation in order to explain the linear temperature dependence of the specific heat at very low temperatures (T < 1 K) [58]. However, as we are interested in temperatures above room temperature, we will not further consider this possibility. Furthermore, the theory we present in the following is purely classical



Figure 11: Same as Figure 10, but now at constant temperature $(125 \,^\circ\text{C})$ with varying stress voltages. Again, the data can be made to overlap. Consequently, the quantity $I_D(t_s) - I_D(1 \,\text{ms})$ is proportional to a temperature and voltage dependent prefactor. This is not necessarily true for the 'real' $\Delta V_{\text{th}}(t_s)$. Nevertheless, this could possibly indicate the dominance of a single (complex) mechanism.

based on the ground-state only. In a possible interpretation of the energy levels, the first transport state may be the anti-bonding (AB) site [59], which has been associated with electrically active trap levels in the silicon bandgap. The anti-bonding site is located behind the Si atom on the other side of the dangling bond. In order to move the hydrogen atom from the dangling bond (DB) to the AB site, lattice relaxation is required, thereby coupling the dissociation process to the silicon-silicon vibrational modes [59].

Upon capture of a carrier, the binding energy is further reduced, thereby favoring complete dissociation of the hydrogen from the silicon dangling bond. In the following we will assume this capture of carriers to happen instantaneously, that is, capture of carriers via quantummechanical tunneling [49] will not be assumed to be ratelimiting. Alternatively, instead of complete dissociation, when the stress is removed, the particle will go back to the ground state, with the time constant determined by the barrier height separating the first transport state from the equilibrium position. Consequently, the energy levels used in the final model may be considered 'effective energy levels', comprising more than a single effect.

Since the gate insulators we are dealing with are amorphous, the barriers separating the ground state from the transport state will be different for each silicon dangling



Figure 12: The energy-levels involved during creation of a dangling bond in an amorphous network, after [60]. Hydrogen is released from a Si–H bond over a barrier into transport states (tetrahedral interstitial sites, bond center sites, etc.). Emission may occur via thermal emission or, at very low temperatures, via tunneling.

bond. For example, with an effective maximum density of interface/oxide states of $10^{12} \dots 10^{13} \text{ cm}^{-2}$, we obtain for a device with a channel length of 100 nm and a width of 1 μ m a total number of possible bonds equal to $N = 10^3 \dots 10^4$, each of which with somewhat different barriers. Experimental support for such a scenario has been given by Stesmans *et al.* [61,62] for both the transition from the ground state to the transport state and back. Also, the fact that interface states at the SiO₂/Si interface show a rather broad Gaussian distribution of energy levels in the silicon bandgap [63] may support the concept of similarly distributed hydrogen binding energies.

For a pure SiO₂ sample, it has been shown that the creation of dangling bonds (Pb centers) directly at the Si/SiO₂ interface is primarily responsible for degradation [64]. In SiON, on the other hand, it has been suggested based on spin-dependent tunneling and recombination measurements that defects are created inside the oxide but still close to the interface, so called K_N centers [52]. These defects have been suggested to also be silicon dangling bonds, but back-bonded to three nitrogen atoms rather than three silicon atoms as in the case of the $P_{\rm b}$ centers. This observation is compatible with the similar degradation kinetics observed in SiO₂ and SiON samples, by placing the common Si-H bond at the heart of the problem. Due to the amorphous nature of SiON, the possible reactions paths may occur in various orientations as shown in Figure 13, a possibility we will make use of to explain PBTI together with mixed NBT/PBT stresses.

It is interesting to note that this approach is very similar to a model successfully used for the description of defect formation and annealing in hydrogenated amorphous silicon [65]. In fact, many of the experimental observations typical for this process seem to have their direct correspondence in bias temperature instabilities (stretched-exponential-like degradation and recovery, considerably better efficiency of holes compared to electrons, etc.)



Figure 13: Schematic distribution of hydrogen bonding sites, possibly K_N centers, in an amorphous nitrided oxide. The orientation of the reaction paths is arbitrary and in most well configurations the DB site is the energetically preferred site.

In order to model the behavior of the system depicted in Figure 13 we should include the ground state, the transition to the first transport state, the transition to the other transport states, and eventually the transition to another ground state after a certain number of 'hops'. However, to study the characteristic features of our model we try to limit the number of energy levels to the absolutely necessary minimum in the following, similarly to the approach taken in [65].

It is also important to realize that previously published NBTI models are in principle fully compatible with this physical picture. However, in the final model formulation of existing models some crucial simplifying assumptions are introduced which may not be justified.

- The reaction-diffusion model [35–37] assumes that the transition rates between the ground state and the first transport state are in equilibrium and that the degradation dynamics are controlled by the redistribution of hydrogen between *identical* transport states (diffusive process).
- 2. Reaction-dispersive-diffusion models [31, 66–68] also assume that the transition rates between the ground state and the first transport state are in equilibrium. By contrast, the degradation dynamics are here controlled by the redistribution of hydrogen between energetically *different* transport states (dispersive-diffusion process). However, the coupling of the distributed transport states to a supposedly fixed ground state and fixed barrier at the interface appears to result in some inconsistencies [68].
- 3. The rate-limited model used by Huard *et al.* [27] assumes that the barrier from the first transport state back to the ground state is so large that practically no re-passivation of the dangling bonds occurs. Such an assumption seems to be a contradiction with the dangling bond being the equilibrium configuration. (The recovery is attributed solely

to hole trapping and detrapping into pre-existing traps.)

2.3 A Double-Well Model

Based on the previous considerations we first investigate a double-well model for BTS, where only the transitions from the ground state to the first transport state (possibly the anti-bonding site) are considered. This is schematically depicted in Figure 14. Application of an electric field is assumed to lower the barrier by an amount of Δ and the second minimum by 2Δ .

Assuming that a particular well is characterized by given barriers V_1 , V_2 , and V_3 , the rate equations describing the depassivation process are then

$$\frac{\partial f_1(t)}{\partial t} = -f_1 k_{13} + f_3 k_{31} , \qquad (12)$$

$$\frac{\partial f_3(t)}{\partial t} = f_1 k_{13} - f_3 k_{31} \tag{13}$$

with the rates given by [56]

$$k_{13}(V_1, V_2) = \nu \exp(-\beta (V_2 - V_1 - \Delta)), \quad (14)$$

$$k_{31}(V_2, V_3) = v \exp(-\beta (V_2 - V_3 + \Delta)). \quad (15)$$

The probability of the hydrogen atom being in well one is given by f_1 , the probability of it being in well 2 f_3 , while having a defect is the probability of the particle not being in well 1, thus $1 - f_1$. Furthermore, we use $1/\beta = k_B T$ and an attempt frequency $v \approx 10^{13} \text{ s}^{-1}$. Obviously, as only energy differences enter the rates, V_1 may be set to zero and eliminated altogether. However, since from a physical point of view each energy may follow a different distribution, the full equation system is retained. We furthermore assume that the individual energy wells are independent and that there is a single hydrogen atom in each well, that is, $f_1 + f_3 = 1$. This assumption may not be justified for unhydrogenated interfaces/oxides or devices with a large background concentration of hydrogen.

Altogether, the threshold voltage shift due to the created defects (assuming instantaneous capture and release of carriers once the defect is created or annealed) is given by the sum of all possible reaction paths and reads

$$\Delta V_{\rm th}(t) = -\frac{q}{C_{\rm ox}} \sum_{i=1}^{N} \left(1 - \Delta f_{i,1}(t) \right) \left(1 - \frac{x_i}{t_{\rm ox}} \right) \,, \quad (16)$$

with $\Delta f_{i,1} = f_{i,1} - f_{i,1}^{eq}$, $f_{i,1}$ the occupancy of the first well in the *i*-th reaction path, $f_{i,1}^{eq}$ its equilibrium value, and x_i the distance from the Si/SiO₂ interface. Assuming that most defects are still close to this interface, we will assume $x_i \approx 0$ in the following (we remark that this approximation can be easily relaxed). Each of the *N* doublewells is then characterized by a unique combination of



Figure 14: A single double-well configuration and the impact of the electric field. In equilibrium, well 1 (V_1) is the energetically preferred configuration. Application of the electric field tilts the wells, in analogy to [56], favoring the second well (V_3). The system is assumed to be positively charged when in the second minimum and the total charge Q is given by the sum over all possible configurations of $(1 - f_1)$. Transitions between the wells are assumed to follow first-order kinetics via thermal activation.

 V_1 , V_2 , and V_3 , which are assumed to be given by independent Gaussian distributions [61, 62]. For computational reasons, however, we will approximate the Gaussian distribution functions using the Fermi-derivative function [27, 69]

$$g_i(V_i, V_{i,m}, \sigma_i) = \frac{1}{\sigma_i} \frac{\exp\left(\frac{V_{i,m} - V_i}{\sigma_i}\right)}{\left(1 + \exp\left(\frac{V_{i,m} - V_i}{\sigma_i}\right)\right)^2} .$$
(17)

Under these approximations it is easy to show that the maximum degradation obtainable in the system is given by

$$\Delta V_{\rm th} \approx -\frac{qN}{C_{\rm ox}} \left(\frac{1}{1 + \exp\left(\frac{V_{3,\rm m} - (V_{1,\rm m} + 2\Delta)}{\sigma_3}\right)} - \frac{1}{\frac{1}{1 + \exp\left(\frac{V_{3,\rm m} - V_{1,\rm m}}{\sigma_3}\right)}} \right).$$
(18)

but a complete analytical solution will be published elsewhere.

2.3.1 Double-Well Model: Relaxation Behavior

The double-well model was calibrated to relaxation data obtained on two different devices at the temperatures 50 °C and 200 °C, see the appendix for experimental details. The calibration to both data sets was performed simultaneously in order to extract physically feasible parameters, see Table 1 for the extracted values. During calibration of the double-well model it was observed that only data recorded at lower temperatures could be well described. Consequently, the weights between the two data sets during calibration were set slightly in favor for



Figure 15: Evaluation of the double-well model (lines) against pMOS recovery data (syms) at two different stress temperatures. While the accuracy at 50 °C is very good, at 200 °C the 'lock-in' is not reproduced, resulting in too fast relaxation.

Parameter	Calibrated Value
σ_2	0.34 eV
σ_3	0.46eV
$V_{2,\mathrm{m}}$	2.53 eV
$V_{3,\mathrm{m}}$	0.09 eV
$\Delta(50^{\circ}C)$	0.60eV
$\Delta(200^{\circ}C)$	0.44 eV

Table 1: The parameters extracted from a simultaneous calibration of the double-well model to relaxation data obtained at 50 °C and 200 °C. Since the voltage applied during relaxation was different at these temperatures (0.34 V @ 50 °C vs. 0.23 V @ 200 °C), Δ was allowed to be temperature-dependent to accommodate this difference. Interestingly, the value for the first barrier height is very close to the value given in literature for the dissociation energy of the Si–H bond (2.4 – 2.6 eV [70]). The same parameter values are of course used for both the stress and relaxation phases in Figure 15 and Figure 16.

the 50 °C data, for which excellent results could be obtained. However, the long logarithmic tails at higher temperatures and larger stress times could not be well reproduced, see Figure 15. This is put down to the emerging 'permanent/slow' component which begins to slow down the relaxation. We were not able to accommodate such a *permanent/slow component*, or, the oft-cited 'lock-in' phenomenon [43], with a double-well model.



Figure 16: Data from the same measurement as in Figure 15 but taken in between the relaxation phases using the OTF approach. The model was calibrated against the relaxation data only. While the basic features are captured, it was not possible to calibrate for the correct amplitude (see the solid lines, which emulate the initial measurement delay of 1 ms and are too low.)

2.3.2 Double-Well Model: Stress Behavior

A comparison of the calibrated double-well model with the data obtained during the intermediate stress phases is shown Figure 16. Although the basic features of the stress data can be captured, the magnitude was found to be too low, which can be traced back to the fact that the double-well model is not able to maintain the logarithmic decay for enough decades and results in a too early rolloff at short relaxation times.

2.4 A Triple-Well Model

As the double-well model cannot accommodate the whole range of experimentally observed features, we include the next transport level (a third well) which accounts for *a more permanent deviation* of the system from its equilibrium configuration. The third well would be separated by a different barrier and could be interpreted as the hydrogen diffusing farther away from the defect (first extension towards a multi-hop limit as suggested in [65]). Such a triple-well model is depicted in Figure 17. Each well is now characterized by a particular combination of V_1 , V_2 , V_3 , V_4 , and V_5 and we have to



Figure 17: Addition of the second transport state results in a triple-well model. The second well is energetically higher than the first and the third well and forms a transitional saddle point. Transitions from the second well back to the first well are fast, while the third well represents the permanent component/lock-in.

solve the linear equation system

$$\frac{\partial f_1}{\partial t} = -f_1 k_{13} + f_3 k_{31} , \qquad (19)$$

$$\frac{\partial f_3}{\partial t} = +f_1 k_{13} - f_3 k_{31} - f_3 k_{35} + f_5 k_{53} , \qquad (20)$$

$$\frac{\partial f_5}{\partial t} = +f_3 k_{35} - f_5 k_{53} . (21)$$

By assuming again that wells do not interact and that there is exactly one hydrogen atom in each well we make use of

$$f_1 + f_3 + f_5 = 1 . (22)$$

The latter assumption seems to be justified as wells without a single hydrogen atom are dangling bonds already, contribute to the initial threshold voltage and will, at least initially, not react to changes in the electric field. By contrast, wells with more than one hydrogen atom will have larger difficulties to react to changes in the field since possible states are already occupied.

The transition rates are modeled in analogy to the double-well model, however, we allow for a different impact of the stress-field on the two wells. The physical picture behind this is that the two barriers are likely to either have a different dipole moment [56, 71], a different tunneling distance, or some other, currently un-

specified, mechanisms which accelerates bond-breaking. Thus, quite generally, we write

$$k_{13} = v \exp(-\beta (V_2 - V_1 - \Delta_2))$$
, (23)

$$k_{31} = v \exp(-\beta (V_2 - V_3 + \Delta_2)), \quad (24)$$

$$k_{35} = v \exp(-\beta (V_4 - V_3 - \Delta_4)). \quad (25)$$

$$k_{53} = v \exp(-\beta(V_4 - V_5 + \Delta_4)), \quad (26)$$

$$k_{53} = v \exp(-p(v_4 - v_5 + \Delta_4))$$
. (20)

In the following, however, we assume that the dispersion of well 1 and well 3 can be neglected, $\sigma_1 = \sigma_5 = 0$, as well as a similar response of the wells to the electric field, $\Delta_2 = \Delta_4$.

2.4.1 Triple-Well Model: Relaxation Behavior

The relaxation behavior predicted by the triple-well model is evaluated against the same data used for the double-well model (cf. Figure 15) in Figure 18. In contrast to the double-well model, the *triple-well model* also reproduces the *permanent component/lock-in* very well which becomes visible at larger stresses.

The extracted parameter values are given in Table 2. Although the model appears to require a large number of parameters, it is important to realize that this is due to the complicated nature of BTI and that for example the latest refined version of the reaction-diffusion model (explicit conversion of H to H₂, diffusion of both species, dynamic occupancy of the interface states [42]) requires an even larger number of parameters without giving comparable accuracy [30].

Parameter	Calibrated Value
σ_2	0.42 eV
σ_3	0.45 eV
σ_4	0.41 eV
$V_{2,\mathrm{m}}$	2.56eV
$V_{3,\mathrm{m}}$	0.80eV
$V_{4,\mathrm{m}}$	3.00eV
$V_{5,\mathrm{m}}$	0.19eV
$\Delta(50^{\circ}C)$	0.47 eV
$\Delta(200^{\circ}C)$	0.38eV

Table 2: The parameters extracted from a simultaneous calibration of the triple-well model to relaxation data obtained at 50°C and 200°C. Note that we assumed $\sigma_1 = \sigma_5 = 0$ and $\Delta_2 = \Delta_4$. The calibrated values for σ_i were very similar, $\sigma_2 \approx \sigma_3 \approx \sigma_4$, and may be substituted by a single parameter. Again, as for the double-well model, the first barrier energy $V_{2,m}$ is in excellent agreement with literature data for the dissociation energy of the Si–H bond.



Figure 18: Evaluation of the triple-well model (solid lines: total, dashed lines: 'permanent' component) against the same data as in Figure 15. For the model evaluation the measurement sequence was simulated using fixed parameters in a single simulation run, just like the real measurement. Excellent accuracy is obtained for both temperatures during the relaxation phase which is not sensitive to mobility changes [72].

2.4.2 Triple-Well Model: Stress Behavior

The prediction of the triple-well model during stress is evaluated in Figure 19 against the OTF data obtained between the relaxation sequences. Note that all data was recorded in a single measurement/stress/measurement sequence. During stress the recorded I_{Dlin} is converted to a threshold voltage shift using the simple on-the-fly expression, $(V_{\text{G}} - V_{\text{th}})\Delta I_{\text{D}}/I_{\text{D0}}$. Recall that this expression is only approximately accurate and prone to overestimation of the real threshold-voltage shift [72].

In particular for moderate stresses, the triple-well model gives excellent agreement during the stress phase, when the impact of the error introduced by the time-zero measurement of I_D is emulated by subtracting $\Delta V_{th}(1 \text{ ms})$ from the simulation data. Quite convincingly, all characteristic features of the data are fully reproduced. For larger stresses, however, a multiplicative offset is observed (a parallel shift in a log-log plot), while the main features of the data are reproduced. We put this down to the mobility variations in the OTF data [53, 72], which have been suggested to produce such an offset for larger stress [42]. Note that ΔV_{th} during relaxation, which is also calculated from I_D using the single point I_D method [73], appears to be insensitive to these errors [72].



Figure 19: Top: The threshold-voltage shift predicted by the triple-well model is also in excellent agreement during each stress phase, at least at 50 °C. Also, the initial delay in the first measurement was taken into account by subtracting $\Delta V_{\text{th}}(1 \text{ ms})$ from the simulation result (shifts the dotted line to the solid line). At higher stresses (temperature or time), the agreement is not that perfect, see the inlay for 200 °C. We put this down to the error in the simple OTF prediction related to mobility degradation and the compact modeling error [53, 72]. **Bottom**: The excellent agreement is confirmed by plotting the individual stress phases on a log scale with the time measured with respect to the beginning of each stress phase.

The occupancy of the second well as a function of the stress time is shown in Figure 20. With increasing stress, the bottom of well 2 is filled, while particles with higher energy are more likely to be transferred to well 3 (the 'permanent' component). Also shown is the impact of a recovery phase which predominantly empties well 2, beginning with the higher-energetic particles.



Figure 20: Top: Occupancy of the individual states in the second well as a function of the energy after the eighth stress phase. **Bottom**: Impact of a 12s relaxation phase on the occupancy. Shown is the impact after the first and the last stress phase.

2.4.3 Triple-Well Model: Duty Factor Dependence

As a next step in the evaluation of the triple-well model, its prediction of the duty-factor (DF) dependency is considered. Available measurement data [34, 47, 74] show a plateau around a DF of about 50% in addition to a strong sensitivity for duty-factors close to 0% and 100%. This issue has been notoriously difficult to model, with the first successful attempt given only recently in [47]. The conventional reaction-diffusion model, for instance, predicts a DF dependence of the form DF^{1/3} [30] and thus no sensitivity for a DF approaching 100%. In particular, RD theory predicts an AC/DC ratio of 80%, see [75], in contrast to the nearly universally observed ratio about 50% [34, 47, 74, 76, 77]. In Figure 21 we show how



Figure 21: The influence of the duty factor on the overall degradation is well reproduced by the triple-well model. The measured degradation is strongly influenced by the measurement delay, 2 ms in our case. Since the period of the oscillation for 10kHz DF stress is much smaller than the measurement delay, the measured degradation does not depend on whether the stress is interrupted for the measurement during the on or off phase (see inlay).

the triple-well model can be used to characterize a *duty-factor dependent stress*. While the agreement is not as perfect as for the relaxation and stress data, the triple-well model correctly predicts the plateau, and the other features of the data.

2.4.4 Triple-Well Model: PBTI Stress

In addition to NBTI, the triple-well model can also be used to describe *PBTI*, see Figure 22, which, remarkably, also generates *positive charge*. However, the degradation and relaxation is not completely symmetric to NBTI [34] in our 1.4 nm SiON samples. In a first attempt, this can be described using different energy barriers in the triplewell model. Whether this is an artifact of the abstract formulation of the barriers where the microscopic origin is left unidentified (the substrate being in inversion or accumulation does so far not enter the model) or a feature of the interfacial layer remains to be investigated.

2.4.5 Triple-Well Model: Mixed NBTI/PBTI Stress

Our current interpretation of the asymmetry relies on the assumption that during PBT stress the same kind of defect is created. For this we assume that the defects responsible for degradation exist with reaction coordinates in two orientations, one parallel and one anti-parallel to the applied electric field, see also Figure 13.



Figure 22: The triple-well model can also be used to describe PBTI stress. However, NBTI and PBTI are apparently asymmetric in our samples, resulting in different parameters of the triple-well model in our current formulation. The two stress bias conditions can be well reproduced using a single parameter set. *Note that PBTI stress also creates positive charge and thus a negative* ΔV_{th} , *just like NBTI*.



Figure 23: Application of a PBTI stress sequence during the relaxation phase after NBTI stress leads to hitherto unexplainable relaxation patterns (data: syms). Using the NBTI-wells calibrated for NBTI stress (Figure 19) and the PBTI-wells calibrated for PBTI stress (Figure 22), these patterns can be straightforwardly explained using superposition (solid lines). In particular, the model explains why large positive biases result in stronger degradation rather than complete recovery as expected from an electron injection model.

Then, upon application of a positive field to the triplewells of Figure 17, the NBTI-wells would not dramatically change their occupancy of well 1. On the other



Figure 24: Detailed view of the recovery after application of small positive bias pulses in between the relaxation sequences. The difference to the normal recovery at $V_G \approx V_{\text{th}}$ is obvious. While the positive bias is too small to trigger a significant response of the PBTI-wells, the occupancy of well 2 of the NBTI-wells is lowered below its equilibrium value, resulting in *degradation* during the 'recovery' phase. The permanent component (that is, the occupancy of well 3, f_5), is given by the dashed line and is insensitive to the small positive bias. Consequently, during CP measurements only f_5 would be visible.

hand, the wells oriented the other way, the PBTI-wells, would start to degrade.

Such an assumption is confirmed when looking at the behavior of a sample first subjected to NBT stress followed by an analogous PBT pattern as used in our NBTI experiments. The most intriguing feature of the NBTIwell/PBTI-well concept is that it allows us to correctly predict the degradation/relaxation behavior of mixed positive/negative stresses. This is demonstrated in Figure 23 where during the relaxation phase after NBTI stress a PBTI stress/relaxation sequence is employed. For small positive bias this leads to an acceleration of recovery. This has previously been explained by assuming the fast component to be due to trapped holes which are annihilated by the injection of electrons at positive biases [27]. However, for *larger positive biases*, the device begins to degrade again, rather than being completely deprived of its recoverable fast component. This appears in contradiction to a hole-trapping theory which assumes a preexisting number of traps. By simply superpositioning the NBTI- and PBTI-wells of Figure 19 and Figure 22, the so-far unexplained stress/relaxation patterns are naturally reproduced and explained.

Also revealing is a look at the detailed recovery pattern after application of positive bias, as shown in Figure 24. After removal of the positive bias, the devices show some small initial degradation, a fact nicely repro-



Figure 25: Occupancy of the individual states in the second well as a function of the energy after the eighth stress phase. After a 12s recovery two cases are considered: (i) 14s additional (conventional) recovery, which causes minimal changes (equal amount of recovery per decade). (ii) 2s recovery at +0.5 V followed by conventional recovery at $V_G = V_{th}$ for 12s. The positive bias dramatically accelerates the recovery and also causes the hydrogen in wells that have the second well as an equilibrium position to move to the first well. Consequently, after application of the positive bias, the occupancy is *lower* than in equilibrium, resulting in an initial degradation when the bias is moved to V_{th} again.

duced by the triple-well model. This can be explained by looking at the simulated occupancy of the second well, see Figure 25, which after application of a positive bias is lowered below its equilibrium value. Restoration of the equilibrium value at $V_{\rm G} = V_{\rm th}$ results in some apparent degradation.

2.4.6 Triple-Well Model: Temperature Scaling

As demonstrated in Figure 10, the experimentally obtained degradation curves, $I_D(t_s) - I_D(1 \text{ ms})$, obtained with the OTF technique at different temperatures can be made to overlap by multiplying each data set with a suitably chosen constant factor. Interestingly, the simulated $\Delta V_{\text{th}}(t_s)$ of the triple-well model do not fulfill this requirement. However, when the OTF measurement is emulated by subtracting the value obtained at 1 ms, a nearly perfect scalability is obtained, see Figure 26. This should again remind us of the dangers when discussing experimental results which always have to be considered in the context of the experimental setup they were obtained with:



Figure 26: Temperature scaling of the triple-well model. After properly emulating the measurement setup, the scaling property is nicely reproduced by the triple-well model.

- Our OTF measurements indicate that the degradation of the drain current $I_D(t_s) - I_D(1 \text{ ms})$ obtained at different temperatures and stress voltages is scalable. *This does not imply that the 'real' drain current shift* $I_D(t_s) - I_D(0 \text{ ms})$ *has to fulfill this property.* Nevertheless, it may indicate the dominance of a single component.
- If the degradation is dominated by a single component, the model does not have to be scalable, that is, it does not necessarily have to be of the form

$$\Delta V_{\rm th}(t_{\rm s}, T, V_{\rm stress}) \approx h(T, V_{\rm stress}) \times \Delta V_{\rm th}(t_{\rm s}) \quad (27)$$

Nevertheless, $\Delta V_{\text{th}}(t_{\text{s}}) - \Delta V_{\text{th}}(t_0)$ should approximately be of that form.

2.5 Conclusion

We have presented a physics-based NBTI/PBTI model derived by considering the individual transitions between possible energetic configurations. In order to find a good compromise between accuracy and efficiency, two approximations were considered in greater detail. The first model just considered a transition between a ground state and an energetically higher state. Models of such kind have for instance been used to explain dielectric relaxation. However, this model was found to be not sufficient to explain NBTI. Inclusion of one additional well, however, considerably improved the accuracy of the model and a detailed and careful evaluation demonstrated that the model is able to describe the degradation during *stress and recovery, positive, negative, and mixed biases*, and the *duty-factor dependence*. The model also gives an intuitive explanation on why fast electrical measurements appear to observe both the fast recovering component on top of a permanent component while charge-pumping experiments only 'see' the permanent part.

2.6 Experimental

The various approximations of our model are evaluated against MSM measurements obtained on pMOSFETs with EOT=1.4 nm [72] in Figure 15. In these MSM measurements we record as much information as possible in a single measurement run [31, 72, 78]:

 On-the-fly (OTF) drain current degradation during exponentially growing stress intervals where eight subsequent stress intervals were used. The degradation of the drain-current is then converted to

$$\Delta V_{\theta} \approx \frac{I_{\rm D} - I_{\rm D0}}{I_{\rm D0}} (V_{\rm G} - V_{\theta 0}) , \qquad (28)$$

a quantity often assumed to have similar properties as the threshold voltage shift ΔV_{th} . In fact, it is now understood that ΔV_{θ} is contaminated by mobility variations and the error in I_{D0} [42, 53, 72], in particular at larger stress times. While the error in I_{D0} , which in our case is determined after 1 ms, can be easily emulated in the simulation, the impact of the mobility variation remains elusive for the time being.

- After each stress interval, in our particular case at 2, 15, 58, 230, 743, 2015, 6008, and 18, 610 s, the gate voltage is switched from the stress voltage to the (temperature-dependent) threshold voltage and the recovery of the drain current is monitored for about 12 s. After the last stress interval, the device is allowed to recover for 10,000 s. The recorded drain current is then converted to a $V_{\rm th}$ shift using an initial $I_{\rm D}V_{\rm G}$ curve (recorded only around the threshold voltage to avoid pre-stressing the device). The first measurement point during recovery was obtained in about 1 ms.
- For Figure 23 and Figure 24, the last long recovery phase was interrupted by positive bias sequences in the same manner as employed during the NBT stress phase.

3 Effect of Strains on Anisotropic Material Transport in Copper Interconnect Structures under Electromigration Stress

We analyzed the effect of strains on material transport in a typical dual damascene copper interconnect via under electromigration stress. The electromigration model incorporates all important driving forces for atom migration coupled with the solution of the electrical and thermal problems. Our approach differs from others by considering a diffusivity tensor in the transport equation taking into account the diffusion anisotropy generated by the applied strains. We have obtained off-diagonal components of the diffusivity tensor up to 30% of the diagonal ones and a different distribution of vacancies due to electromigration.

3.1 Introduction

Electromigration is the transport of material caused by the momentum transfer between conducting electrons and metal atoms [79]. With the continuous shrinking of the dimensions of modern integrated circuits the interconnects become subjected to higher current densities. In addition, the interconnect structure can be arranged in up to ten levels of wiring with thousands of interlevel connections such as vias. Hence, failure of metallic interconnect caused by electromigration is a key issue for reliability in microelectronics and the prediction of the long term interconnect behavior has become a major issue. The theoretical models of electromigration have gone through a long evolution starting with the early works of Black [79], Rosenberg and Ohring [80], Blech et al. [81-83], Kirchheim et al. [84], Korhonen et al. [10], Lloyd et al. [85, 86], and Clement [87], to the more general contemporary models of Sarychev et al. [88] and Sukharev [15].

Electromigration can be viewed as a multi-physics phenomenon, once the material transport is caused by several driving forces, such as concentration gradient, electric field, temparature gradient, and mechanical stress [88]. Residual mechanical stresses are introduced on interconnect lines as a result of the fabrication process flow [89]. Copper interconnects are typically produced by a dual damascene process, for which surrounding cap and barrier layers are mandatory. The choice of passivating film material together with the corresponding technology process produce tensile or compressive stresses in the interface between the passivating film and the interconnect metal. These stresses can be very high [90] leading to a significant anisotropic diffusion of the metal atoms [91].

In this work we evaluate the changes in the electromigration material transport in three-dimensional typical copper interconnect structures due to the anisotropic diffusivity of vacancies produced by residual strains, taking into account all relevant driving forces for atom migration.

3.2 Electromigration Modeling

The total vacancy flux caused by the gradients of concentration, electrical potential, temperature, and mechanical stress, respectively, is given by [88]

$$\vec{J_{\nu}} = -\mathbf{D} \bigg(\nabla C_{\nu} + \frac{Z^* e}{kT} C_{\nu} \nabla \varphi - \frac{Q^*}{kT^2} C_{\nu} \nabla T + \frac{f\Omega}{kT} C_{\nu} \nabla \sigma \bigg), \qquad (29)$$

where **D** is the diffusivity tensor, C_v is the vacancy concentration, Z^*e is the effective charge, Q^* is the heat of transport, $f\Omega$ is the vacancy volume relaxation, σ is the hydrostatic stress, *k* is Boltzmann's constant, and *T* is the temperature.

In conjunction with (29) the dynamics of the vacancies is obtained by solving the mass balance equation

$$\frac{\partial C_{\nu}}{\partial t} = -\nabla \cdot \mathbf{J}_{\nu} + G(C_{\nu}), \qquad (30)$$

with

$$G(C_{\nu}) = -\frac{C_{\nu} - C_{\nu}^{eq}}{\tau}, \qquad (31)$$

where $G(C_v)$ is a source function introduced by Rosenberg and Ohring [80], which models the vacancy annihilation and generation processes, and τ is the characteristic relaxation time [15].

The diffusivity tensor **D** is calculated by [91]

$$D_{ij} = \frac{1}{2} \sum_{k=1}^{12} R_i^k R_j^k \Gamma^k,$$
(32)

where \vec{R}^k is the jump vector for a site *k* and Γ^k is the jump rate. The impact of the strains is a change of the jump rate through [92]

$$\Gamma^{k} = \Gamma_{0} \exp\left[\frac{-\Omega \vec{\varepsilon}_{I} \cdot (\mathbf{C} \, \vec{\varepsilon})}{kT}\right],\tag{33}$$

where $\vec{\epsilon}_I$ is the induced strain, $\vec{\epsilon}$ is the applied strain, and **C** is the elasticity tensor of the interconnect material. Due to the symmetry of a vacant point defect the induced strain is determined by

$$\varepsilon_I = -\frac{1-f}{3},\tag{34}$$

and the final induced strain vector is determined by

$$\vec{\varepsilon}_I = \varepsilon_I \mathbf{r}^k,$$
 (35)

where \mathbf{r}^k is a unit vector in the jump direction for a site k.

The simulation procedure is shown in Figure 27. First, the electro-thermal problem determines the electric potential and the temperature distribution in the interconnect geometry, which are transferred to the electromigration model. Due to the fabrication process it is expected that anisotropic strains in the order of 0.1% to 1% [90, 93] have developed in the interconnects. We have set similar strains into $\vec{\epsilon}$ in equation (33) to reproduce the expected anisotropy. Therefore, the solution of the electromigration problem provides the vacancy distribution for each specific set of strains. Both the electro-thermal problem and the electromigration model are solved numerically by the finite element method [94] implemented in an in-house code.



Figure 27: The simulation procedure.



Figure 28: Interconnect via geometry showing the metal line, capping layer, and barrier layer.

3.3 Simulation Results

The interconnect geometry analyzed by fully threedimensional simulation is given in Figure 28. The structure is an idealized via as produced by a dual damascene



Figure 29: Electric potential distribution.



Figure 30: Vacancy concentration for the interconnect without strains (units in cm^{-3}). The higher vacancy concentration on the interface between the bottom copper line and the etch stop layer occurs due to the increased interfacial diffusion coefficient.

process for copper as interconnect metal. In order to avoid the copper to move into the interlevel passivation (not shown in figure), a capping layer is used, typically of SiN. The barrier layer serves also as a redundant path for electrical conduction. The line and via have a cross section of 0.2 x 0.2 μm^2 , the tantalum barrier and capping layers are 20 nm thick. For the electromigration calculation we have assumed that the vacancy flux vanishes at the anode and cathode end of the interconnect structure, which corresponds to a blocking boundary condition.

In Figure 29 we show the electric potential distribution. The applied current density is $2MA/cm^2$ in the *x* direction, i.e. the electrons flow from the bottom line up to the via and the upper line.

Considering initially that the interconnect is free of strains, i.e. $\vec{\epsilon}$ in (33) vanishes, we obtained the vacancy distribution as shown in Figure 30, with $10^{16}cm^{-3}$ used as the initial vacancy concentration for copper [10]. This corresponds to the case of isotropic diffusion and the diffusivity tensor is a diagonal matrix with equal entries. As expected, the vacancies concentrate "downstream",



Figure 31: Vacancy concentration for the residual strains $\varepsilon_{xx} = 0.010, \varepsilon_{yy} = 0.005$ and $\varepsilon_{zz} = 0.001$ (units in cm^{-3}).

mainly in the via region, where the copper meets the barrier layer, with a small increase above the initial concentration.

It is well known that the interface between the copper and capping layer can act as a fast diffusivity path for atom migration. In order to consider that in our simulations we have increased the diffusion coefficient in this region, following the same approach as made by Sukharev [15]. The result is also a higher vacancy concentration in the cathode on the interface between the bo



Figure 33: Vacancy concentration as a function of the distance from top to bottom of the upper metal line at the center of the via.

Applying the strains $\varepsilon_{xx} = 0.010$, $\varepsilon_{yy} = 0.005$ and $\varepsilon_{zz} = 0.001$, we have verified only a very small increase in the vacancy concentration on the bottom of the via, as depicted in Figure 31. The maximum vacancy concentration increased to $1.07 \times 10^{16} cm^{-3}$. In this case we have determined the off-diagonal components of the diffusivity tensor to be about 18% of the diagonal ones.

Considering $\varepsilon_{xx} = 0.008$, $\varepsilon_{yy} = 0.015$ and $\varepsilon_{zz} = 0.003$ the distribution of vacancies is significantly altered, as Figure 32 shows, although the change in the maximum



Figure 32: Vacancy concentration for the residual strains $\varepsilon_{xx} = 0.008, \varepsilon_{yy} = 0.015$ and $\varepsilon_{zz} = 0.003$ (units in cm^{-3}).

concentration to $1.08 \times 10^{16} cm^{-3}$ is still small. We have observed a drift of vacancies in the *z* direction and, consequently, an accumulation to the right edge of the interconnect in relation to the direction of the electric current. The higher strains applied in equation (33) increased the off-diagonal diffusion coefficients in relation to the diagonal values. According to (32), we have determined $\frac{D_{ij,i\neq j}}{D_{ii}}$ to be about 30%. The differences in the material distribution presented by the previous pictures is more easily seen in Figure 33, which shows the vacancy concentration along a cut line from top to bottom in the upper interconnect line at the center region of the via.

3.4 Conclusion

The effect of strains on material transport in a typical dual damascene copper interconnect via under electromigration stress has been analyzed. The model incorporates all important driving forces for atom migration. Although in a fcc metal, like copper, the diffusivity is isotropic, the residual strains affect the jump rate of atoms to a vacant point effect producing an anisotropy in the diffusion. A diffusivity tensor in the transport equation takes into account this anisotropy generated by the applied strains. No change is observed in the vacancy distribution, until strains on the order of 0.5% to 1% are used. The maximum vacancy concentration cannot increase so much in relation to the equilibrium value, although the higher strains result in significant changes in the off-diagonals components of the diffusivity tensor. This can lead to significant anisotropy of material transport in an interconnect line under electromigration stress and this effect must be taken into account for a rigorous analysis of the electromigration problem.

4 Current Transport in Carbon Nanotube Transistors

Carbon nanotubes (CNTs) have been studied in recent years due to their exceptional electronic, opto-electronic, and mechanical properties. To explore the physics of carbon nanotube field-effect transistors (CNT-FETs) self-consistent quantum mechanical simulations have been performed. The performance of carbon nanotubebased transistors is analyzed numerically, employing the non-equilibrium Green's function formalism. Electronphonon interaction parameters, such as electron-phonon coupling strength and phonon energy, strongly depend on the chirality and the diameter of the carbon nanotube. The steady-state and the dynamic response of carbon nanotube based transistors are studied for a wide range of electron-phonon interaction parameters.

4.1 Introduction

Novel structures and materials such as multiple gate MOSFETs, carbon nanotube field-effect transistors (CNT-FETs), and molecular based transistors, are expected to be introduced to meet the requirements for scaling [95]. CNTs can be considered as a graphene sheet which has been wrapped into a tube. The way the graphene sheet is wrapped is represented by a pair of indices (n,m) called the chiral vector. The integers n and *m* denote the number of unit vectors along two directions in the honeycomb crystal lattice of graphene. If m = 0, the CNT is called *zigzag*. If n = m, the CNT is called armchair. Otherwise, it is called chiral. CNTs with n-m=3 are metals, otherwise they are semiconductors [96]. Semiconducting CNTs can be used as channels for transistors [97], and metallic CNTs can serve as interconnect wires [98].

CNT-FETs have been considered in recent years as potential alternatives to CMOS devices due to their excellent electronic properties [99, 100]. Some of the interesting electronic properties of CNTs are quasi-ballistic carrier transport [101], suppression of short-channel effects due to one-dimensional electron transport [102, 103], and nearly symmetric structure of the conduction and valence bands [104], which is advantageous for complementary circuits. Moreover, owing to excellent optical properties of CNTs, an all-CNT electronic and optoelectronic devices can be envisioned. The direct bandgap and the tunability of the band-gap with the CNT diameter renders them as suitable candidates for optoelectronic devices, especially for infra-red (IR) applications [105, 106] due to the relatively narrow band gap.

The non-equilibrium Green's function (NEGF) method has been successfully utilized to investigate

the characteristics of nano-scale silicon transistors [107–109], CNT-FETs [110–118], and molecular devices [119–124]. In this work we discuss the NEGF formalism to study quantum transport in CNT-FETs.

The outline of the paper is as follows. In Section 4.2, the NEGF formalism is briefly described. The implementation of this method for CNT-FETs is presented in Section 4.3. The electron-phonon interaction parameters of a CNT depend on the chiral vector, which implies that many different parameter values exist. In Section 4.4 the device response is studied for a wide range of electron-phonon interaction parameters. After a brief discussion in Section 4.6 conclusions are presented in Section 4.7.

4.2 Non-equilibrium Green's Function Formalism

The NEGF formalism initiated by Schwinger, Kadanoff, and Baym allows to study the time evolution of a manyparticle quantum system. Knowing the single-particle Green's functions of a given system, one may evaluate single-particle quantities such as carrier density and current. The many-particle information about the system is cast into self-energies, which are part of the equations of motion for the Green's functions. A perturbation expansion of the Green's functions is the key to approximate the self-energies. Green's functions enable a powerful technique to evaluate the properties of a manybody system both in thermodynamic equilibrium and non-equilibrium situations.

Four types of Green's functions are defined as the nonequilibrium statistical ensemble averages of the single particle correlation operator [125]. The greater Green's function $G^>$ and the lesser Green's function $G^<$ deal with the statistics of carriers. The retarded Green's function G^R and the advanced Green's function G^A describe the dynamics of carriers.

$$G^{>}(1,2) = -i\hbar^{-1} \langle \hat{\psi}(1) \hat{\psi}^{\dagger}(2) \rangle$$

$$G^{<}(1,2) = +i\hbar^{-1} \langle \hat{\psi}^{\dagger}(2) \hat{\psi}(1) \rangle$$

$$G^{R}(1,2) = \theta(t_{1}-t_{2})[G^{>}(1,2) - G^{<}(1,2)]$$

$$G^{A}(1,2) = \theta(t_{2}-t_{1})[G^{<}(1,2) - G^{>}(1,2)]$$
(36)

The abbreviation $1 \equiv (\mathbf{r}_1, t_1)$ is used, $\langle \dots \rangle$ is the statistical average with respect to the density operator, $\theta(t)$ is the unit step function, $\hat{\psi}^{\dagger}(\mathbf{r}_1, t_1)$ and $\hat{\psi}(\mathbf{r}_1, t_1)$ are the field operators creating or destroying a particle at point (\mathbf{r}_1, t_1) in space-time, respectively. The Green's functions are all correlation functions. For example, $G^>$ relates the field operator $\hat{\psi}$ of the particle at point (\mathbf{r}_1, t_1) in space-time to the conjugate field operator $\hat{\psi}^{\dagger}$ at another point (\mathbf{r}_2, t_2) .

4 Current Transport in Carbon Nanotube Transistors

Under steady state condition the Green's functions depend only on time differences. One usually Fourier transforms the time difference coordinate, $\tau = t_1 - t_2$, to energy. For example, the lesser Green's function is transformed as $G^{<}(1,2) \equiv G^{<}(\mathbf{r_1},\mathbf{r_2};E) = \int (d\tau/\hbar)e^{iE\tau/\hbar}G^{<}(\mathbf{r_1},\mathbf{r_2};\tau)$.

Under steady-state condition the equation of motion for the Green's functions can be written as [126]:

$$[E - H] G^{\text{R},\text{A}}(1,2) - \int d3 \, \Sigma^{\text{R},\text{A}}(1,3) G^{\text{r},\text{a}}(3,2) = \delta_{1,2}$$
(37)
$$G^{\lessgtr}(1,2) = \int d3 \int d4 \, G^{\text{R}}(1,3) \Sigma^{\lessgtr}(3,4) G^{\text{A}}(4,2)$$
(38)

where *H* is the single-particle Hamiltonian operator, and Σ^{R} , $\Sigma^{<}$, and $\Sigma^{>}$ are the retarded, lesser, and greater selfenergies, respectively.

4.3 Implementation

This section describes the implementation of the outlined NEGF formalism for the numerical analysis of CNT-FET. Figure 34 shows the structure of the simulated device. A tight-binding Hamiltonian is used to describe



Figure 34: Cross section of the investigated CNT based transistor and the band-edge profile at the source sided metal-CNT interface. Depending on the work function difference between metal and CNT, a positive, zero, or negative barrier height for electrons or holes can be achieved.

transport phenomena in CNT-FETs. The self-energy due to electron-phonon interactions are studied next.

4.3.1 Tight-Binding Hamiltonian

In Graphene three σ bonds hybridize in an sp^2 configuration, whereas the other $2p_z$ orbital, which is perpendicular to the graphene layer, forms π covalent bonds. The π energy bands are predominantly determining the solid state properties of graphene. Similar considerations hold for CNTs. We use a nearest-neighbor tight-binding π -bond model [127]. Each atom in an sp^2 -coordinated CNT has three nearest neighbors, located $a_{cc} = 1.42$ Å away. The band-structure consists of π -orbitals only, with the hopping parameter $t = V_{pp\pi} \approx -2.7$ eV and zero on-site potential.

The tight-binding Hamiltonian matrix for a (n,0) zigzag CNT, shown in Figure 35-a, can be written



Figure 35: Layer layout of a (n,0) zigzag CNT. a) The coupling matrices between layers are denoted by $t_{\underline{1}}$ and $t_{\underline{2}}$, where $t_{\underline{1}}$ is a diagonal matrix and $t_{\underline{2}}$ includes off-diagonal elements. b) The corresponding one-dimensional chain, in mode space, with two sites per unit cell with hopping parameters t and $t_{\underline{2}}^{v} = 2t \cos(\pi v/n)$.

as [127]

$$\underline{H} = \begin{pmatrix} \underline{U}_{1} & \underline{t}_{1} & & & \\ \underline{t}_{1} & \underline{U}_{2}^{\dagger} & \underline{t}_{2} & & & \\ & \underline{t}_{2}^{\dagger} & \underline{U}_{3} & \underline{t}_{1} & & \\ & & \underline{t}_{1} & \underline{U}_{4} & \underline{t}_{2}^{\dagger} & \\ & & & \underline{t}_{2} & \underline{U}_{5} & \\ & & & & & \ddots \end{pmatrix}$$
(39)

where the underlined quantities denote matrices. We assume that the electrostatic potential shifts the on-site potential. Therefore, U_i is a diagonal matrix which represents the electrostatic potential energy in the *i*th circumferential ring of carbon atoms. Equal electrostatic potential for all carbon atoms within a ring is assumed, therefore $U_i = U_i I$. The first and second kind of interaction matrix between the neighboring rings are denoted by t_1 and t_2 . Only the nearest neighbor interaction between carbon atoms is considered. The coupling matrix between layer 2 and layer 3 is diagonal, $t_1 = t I$, where t is the hopping parameter. However, the coupling matrix between layer 1 and layer 2 is given by

$$\underline{t_2} = \begin{pmatrix} t & t \\ t & t \\ & t & t \\ & & \ddots \end{pmatrix}$$
(40)

The eigen vectors of the matrix t_2 represent plane waves around the circumference of the CNT with the quantized wave-vectors $k_v = 2\pi v/\sqrt{3}a_{cc}n$, where v =1,2,...n [127], and the eigen values $2t \cos(\pi v/n)$. By transforming from real space into eigen mode space [128], the subbands become decoupled and the Hamiltonian can be written as $\underline{H} = \sum_v \underline{H}^v$, where \underline{H}^v , the Hamiltonian of the subband v, is given by

$$\mathbf{H}^{\mathbf{v}} = \begin{pmatrix} U_{1}^{\mathbf{v}} & t_{1}^{\mathbf{v}} & & & \\ t_{1}^{\mathbf{v}} & U_{2}^{\mathbf{v}} & t_{2}^{\mathbf{v}} & & & \\ & t_{2}^{\mathbf{v}} & U_{3}^{\mathbf{v}} & t_{1}^{\mathbf{v}} & & \\ & & t_{2}^{\mathbf{v}} & U_{4}^{\mathbf{v}} & t_{2}^{\mathbf{v}} \\ & & & t_{1}^{\mathbf{v}} & U_{4}^{\mathbf{v}} & t_{2}^{\mathbf{v}} \\ & & & & t_{2}^{\mathbf{v}} & U_{5}^{\mathbf{v}} & . \\ & & & & & & . & . \end{pmatrix}, \quad (41)$$

where $U_i^v = U_i$, $t_1^v = t$, and $t_2^v = 2t \cos(\pi v/n)$ [117,127]. The one-dimensional tight-binding Hamiltonian \underline{H}^v describes a chain with two sites per unit cell with on-site potential U_i^v and hopping parameters t and t_2^v , see Figure 35-b.

4.3.2 Electron-Phonon Self-Energies

Because in the CNT two degrees of freedom are confined, an electron can only be scattered forward or backward in the axial direction, preserving or changing the sign of the band-velocity, respectively. We assume bias conditions for which the first subband predominantly contributes to the total current and only intra-subband intra-valley transitions have to be considered.

A linear dispersion relation for acoustic phonons is assumed, $\omega_{q,\lambda} \approx v_{\lambda}|q|$, where v_{λ} is the acoustic phonon velocity and λ is the phonon polarization. For optical phonons the energy is assumed to be independent of the phonon wave-vector $\omega_{q,\lambda} \approx \omega_{\text{OP},\lambda} = \text{const.}$ Similarly, the matrix elements of electron-phonon interaction [129] can be approximated as $M_{q,\lambda} \approx M_{\lambda}^{\text{AP}}|q|$ for acoustic phonons and $M_{q,\lambda} \approx M_{\lambda}^{\text{OP}} = \text{const}$ for optical phonons. The interaction of electrons with optical phonons is inelastic. Assuming that the electron-phonon interaction occurs locally [130] the self-energies can be written as

$$\begin{split} \Sigma_{\text{inel}}^{<,\nu}(E) &= \sum_{\lambda} D_{\text{inel},\lambda} \\ \times [(N_{\lambda}+1) \, G^{<,\nu}(E+\hbar\omega_{\lambda}) + N_{\lambda} G^{<,\nu}(E-\hbar\omega_{\lambda})] \\ (42) \\ \Sigma_{\text{inel}}^{>,\nu}(E) &= \sum_{\lambda} D_{\text{inel},\lambda} \\ \times [(N_{\lambda}+1) \, G^{>,\nu}(E-\hbar\omega_{\lambda}) + N_{\lambda} G^{>,\nu}(E+\hbar\omega_{\lambda})] \end{split}$$

where N_{λ} is the phonon occupation number which is given by the Bose-Einstein distribution function. The electron-phonon interaction strength is given by

$$D_{\text{inel},\lambda} = \frac{\hbar |M_{\lambda}^{\text{OP}}|^2}{2nm_c \omega_{\lambda}}$$
(44)

(43)

where m_c is the mass of a carbon atom. The first term in (42) corresponds to the emission of a phonon by the de-excitation of an electron and the second term corresponds to the excitation of an electron by the absorption of a phonon. Interaction with acoustic phonons can be regarded as elastic scattering, $E \pm \hbar \omega_{\lambda} \approx E$, and the approximation $N_{\lambda} \approx N_{\lambda} + 1 \approx k_{\rm B}T/\hbar v_{\lambda}$ can be used. Based on this approximation, the self-energies for acoustic phonon interaction simplify to

$$\Sigma_{\rm el}^{\leq,\nu}(E) = D_{\rm el}^{\nu} G^{\leq,\nu}(E) \tag{45}$$

$$D_{\mathrm{el},\lambda} = \frac{k_{\mathrm{B}}T |M_{\lambda}^{\mathrm{AP}}|^2}{nm_{\mathrm{c}}\upsilon_{\lambda}}$$
(46)

The self-energy due to electron-phonon interaction comprises the contributions of elastic and inelastic scattering mechanisms, $\Sigma_{e-ph}^{\nu} = \Sigma_{el}^{\nu} + \Sigma_{inel}^{\nu}$. The transport equations must be iterated to achieve convergence of the electronphonon self-energies, resulting in a self-consistent Born approximation.

4.3.3 Self-Consistent Simulations

To solve transport equations numerically they need to be discretized in both the spatial and the energy domain. The carrier concentration at some node l of the spatial grid and the current density at the edge between the nodes l and l + 1 are given by

$$n_{l} = -4i \sum_{\nu} \int \frac{dE}{2\pi} G_{l,l}^{<,\nu}(E)$$
 (47)

$$j_{l,l+1} = \frac{4q}{\hbar} \sum_{\nu} \int \frac{dE}{2\pi} 2\Re e\{G_{l,l+1}^{<,\nu}(E)t_{l+1,l}^{\nu}\}$$
(48)

where the factor 4 is due to the spin and band degeneracy.

For an accurate analysis it is essential to solve the coupled system of transport equations and the Poisson equation self-consistently [124]. The convergence of the selfconsistent iteration is a critical issue. To achieve convergence, fine resonances at some energies in (47) have to be resolved accurately. For that purpose an adaptive method for selecting the energy grid is essential [131].

4.4 The Effect of Electron-Phonon Interaction

The electron-phonon coupling strength and the phonon energy depend on the chirality and the diameter of the CNT [129]. In this section the device response is studied for a wide range of electron-phonon interaction parameters.

4.5 Electron-Phonon Coupling Strength

Figure 36-a shows the ballisticity as a function of the electron-phonon coupling strength. The ballisticity is defined as $I_{\rm Sc}/I_{\rm Bl}$, the ratio of the on-current in the presence of electron-phonon interaction to the current in the ballistic case [132].

The left part of Figure 36-b illustrates an electron losing its kinetic energy by emitting a phonon. The electron



Figure 36: a) Ballisticity versus electron-phonon coupling strength for a CNT of 50 nm length. Results for both elastic and inelastic scattering with different phonon energies are shown. The operating point is $V_{\rm G} = V_{\rm D} = 1$ V. b) Sketch of phonon emission and absorption processes in the channel.

will be scattered either forward or backward. In the case of backward scattering the electron faces a thick barrier near the source contact and will be reflected with high probability, such that its momentum will again be directed towards the drain contact.

Elastic scattering conserves the energy of carriers, but the current decreases due to elastic back-scattering of carriers. Figure 37-a shows that for elastic scattering the source and drain current spectra are symmetric. As the electron-phonon coupling strength increases, resonances in the current spectrum are washed out and the total current decreases due to elastic back-scattering. In the case of inelastic scattering, carriers acquiring enough kinetic energy can emit a phonon and scatter into lower energy states. Therefore, as shown in Figure 37-b, the source and drain current spectra are not symmetric. As the coupling strength increases more electrons are scattered into lower energy states.

4.5.1 Phonon Energy

Figure 38-a shows the dependence of the ballisticity with respect to the phonon energy. With increasing phonon energy the effect of phonon scattering on the current is reduced, because scattered electrons lose more kinetic energy and the probability for traveling back to the source contact decreases. The considerable decrease of ballisticity for low energy phonons is due to the phonon absorption process. The right part of Figure 36-b shows an electron absorbing energy from a phonon and scattering into a higher energy state. In this case, the probability for arriving at the source contact increases. This process can severely reduce the total current.

Figure 38-b separately shows the effects of the phonon emission and absorption processes on the ballisticity. As the phonon energy decreases, the phonon occupation number increases exponentially, and the self-energy contributions of these two components increase. However, due to the higher probability for back-scattering of electrons in the case of phonon absorption, this component reduces the total current more effectively than the phonon emission process does.

4.5.2 Switching Response

To illustrate the effect of electron-phonon interaction on the dynamic response of the device, the gate-delay time defined as $\tau = (Q_{\rm on} - Q_{\rm off})/I_{\rm on}$ [133] is considered, where the quasi static approximation is assumed. It has been shown that the quasi static approximation for CNT based transistors is justified for frequencies below THz [134].

Figure 39-a shows the ratio of the gate-delay time in the ballistic case to that in the presence of electronphonon interaction, τ_{BI}/τ_{Sc} , as a function of the electronphonon coupling strength. As the phonon energy increases the gate-delay time increases. This behavior can be attributed to the average electron velocity in the channel, which is high for ballistic electrons and low for electrons scattered to lower energy states.

Figure 39-b shows the spectra of the source and drain currents for different inelastic phonon energies. Electrons can emit a single phonon or a couple of phonons to reach lower energy states. The probability of multiple phonon emissions decreases as the number of interactions increases. Therefore, as the phonon energy



Figure 37: The spectra of the source and drain currents. a) The effect of elastic phonon scattering with different coupling strengths is shown. b) The effect of inelastic phonon scattering with different coupling strengths is shown. The phonon energy is $\hbar\omega = 100$ meV.



Figure 38: a) Ballisticity versus phonon energy for a CNT of 50 nm length. Results for inelastic scattering with different electron-phonon couplings are shown. $V_{\rm G} = V_{\rm D} = 1$ V. b) Ballisticity versus phonon energy with $D = 10^{-1}$ eV² at the bias point $V_{\rm G} = V_{\rm D} = 1$ V. The contributions due to phonon absorption and emission are shown.

increases, the occupation of electrons at lower energy **4.5.3** states increases.

As shown in Figure 39-b, the electron population close to the conduction band-edge considerably increases as the phonon energy increases. Therefore, as the phonon energy increases the mean velocity of electrons decreases and the carrier concentration in the channel increases (Figure 40). The increased charge in the channel results in an increased gate-delay time.

4.5.3 Diffusive Limit

All the above discussed results were obtained for a device with a CNT length of 50 nm. In the case of ballistic transport the current is independent of the device length, but in the presence of scattering it decreases as the device length increases. Figure 41-a shows the ballisticity as a function of the CNT length in the presence of elastic and inelastic electron-phonon interaction. An artificially large value for the electron-phonon coupling strength and a small value for the phonon energy is cho-



Figure 39: a) The ratio of the gate-delay time in the ballistic case to that in the presence of electron-phonon interaction. For comparison, the ratio I_{Sc}/I_{B1} is also shown. b) The spectra of the source and drain currents. The effect of inelastic scattering with different phonon energies is shown. The electron-phonon coupling strength is $D = 2 \times 10^{-1} \text{ eV}^2$. A considerable increase of the electron population close to the conduction band-edge as the phonon energy increases is visible.



Figure 40: a) The profile of the electron velocity near the source contact. b) The profile of the electron concentration along the device. The results for the ballistic case and for electron-phonon interaction are shown. As the phonon energy increases the electrons scatter to lower energy states. Therefore, the electron velocity decreases and the carrier concentration increases. The electron-phonon coupling strength is $D = 10^{-1} \text{ eV}^2$ and the bias point is $V_G = V_D = 1 \text{ V}$.

sen to simulate the diffusive limit (see Figure 41-b). In this case the current is expected to be inversely proportional to the device length according to Ohm's law.

4.6 Discussion

In general the electron-phonon interaction parameters depend on the diameter and the chirality of the CNT [129]. CNTs with a diameter $d_{\text{CNT}} > 2$ nm have a band gap $E_{\rm G} < 0.4$ eV, which render them unsuitable as channel for transistors. Since the fabrication of devices with a diameter $d_{\rm CNT} < 1$ nm is very difficult, we limit our study to zigzag CNTs with diameters in the range of $d_{\rm CNT} = 1 - 2$ nm.

Scattering with acoustic phonons is treated as an elastic process. The electron-phonon coupling is also weak for acoustic phonons ($D_{\rm AP} < 10^{-3} \, {\rm eV}^2$), which implies that elastic back-scattering of carriers is weak. Inelastic



Figure 41: a) Ballisticity versus CNT length. The electron-phonon coupling strength for both elastic and inelastic scattering is $D = 10^{-1} \text{ eV}^2$, and $\hbar \omega = 25 \text{ meV}$ for inelastic scattering. These scattering parameters simulate the diffusive regime. In this case the ballisticity is inversely proportional to the device length [135]. b) Ballisticity as a function of the electron-phonon coupling strength and phonon energy for inelastic scattering. The scale of the ballisticity is shown in the side bar. The regions of ballistic and diffusive transport are shown. As the strength of the electron-phonon interaction increases transport of carriers deviates from the ballistic limit and becomes more diffusive.



Figure 42: Comparison of the simulation results and experimental data for the a) output and b) transfer characteristics. Lines show the simulation results and symbols show experimental data. The result for $V_{\rm G} = -1.3$ V is compared with the ballistic limit. Experimental data have been adopted from [136].

tic scattering is induced by optical (OP), radial breathing mode (RBM), and K-point phonons [104, 137]. Considering the class of CNTs discussed above, energies of these phonons are $\hbar\omega_{OP} \approx 200 \text{ meV}$, $\hbar\omega_{RBM} \approx 25 \text{ meV}$, and $\hbar\omega_{K_1} \approx 160 \text{ meV}$ and $\hbar\omega_{K_2} \approx 180 \text{ meV}$ [132, 137]. The corresponding coupling coefficients are $D_{OP} \approx 40 \times 10^{-3} \text{ eV}^2$, $D_{RBM} \approx 10^{-3} \text{ eV}^2$, and $D_{K_1} \approx 10^{-4} \text{ eV}^2$, and $D_{K_2} \approx 10^{-3} \text{ eV}^2$ [132]. As discussed in Section 4.5.1, high energy phonons such as OP and K-point phonons reduce the on-current only weakly, but can increase the gate-delay time considerably due to charge pileup in the channel. Low energy phonons such as the RBM phonon can reduce the on-current more effectively, but have a weaker effect on the gate-delay time. However, due to strong coupling, scattering processes are mostly due to electronphonon interaction with high energy phonons. Therefore, at room temperature the on-current of short CNT-FETs can be close to the ballistic limit [136] (see Figure 42), whereas the gate-delay time can be significantly below that limit [138–140].

The intrinsic (without parasitic capacitances) gatedelay time for the ballistic case can be approximated as $\tau \approx 1.7$ ps/ μ m, or equivalently $f_T \approx$ 100 GHz/ μ m [133]. The highest reported intrinsic cutoff frequency for a device with a length of 300 nm is $f_T \approx 30$ GHz [141], which is far below the ballistic limit. Inelastic electron-phonon interaction with high energy phonon has to be considered to explain the results.

4.7 Conclusion

The coupled system of transport and Poisson equations was solved self-consistently. A tight-binding Hamiltonian is used to describe transport phenomena in CNT-FETs. Employing the described model, both the static and dynamic response of CNT-FETs was investigated. The effect of electron-phonon interaction on the device characteristics is discussed in detail. In agreement with experimental data, our results indicate that at room temperature electron phonon interaction affects the steadystate current of CNT-FETs only weakly, whereas the switching response of such devices can be significantly affected.

5 Modeling of Macroscopic Transport Parameters in Inversion Layers

We present a parameter extraction technique for higherorder transport models for a 2D electron gas in ultra thin body SOI MOSFETs. To describe 2D carrier transport we have developed a self consistent Schrödinger-Poisson Subband Monte Carlo simulator. The method takes into account quantization effects and a non equilibrium distribution function of the carrier gas, which allows an accurate description of the parameter behavior for high electric fields. Finally the results are compared with the transport parameters of 3D bulk electrons and the influence of the channel thickness on the mobility is investigated.

5.1 Introduction

As the dimensions of modern semiconductor devices have reached the deca-nanometer regime, the driftdiffusion model, which is still the workhorse of today's TCAD tools, becomes more and more inaccurate [142]. Promising results have been obtained from higher-order transport models systematically derived from Boltzmann's equation [143] which can cover the important gate-length range down to about 25 nm [142]. An advantage of the drift-diffusion model is that it contains only one transport parameter, the carrier mobility which can be taken from measurement. For the energy-transport model and the six moments model additional parameters have to be supplied. However modeling of these transport parameters is highly critical. So far, these parameters have been determined using bulk Monte Carlo simulations and successfully used in table-based macroscopic transport models for nin-structures [143]. However, since the transport parameters are fundamentally affected by the surface properties and quantization in the inversion layer of ultra-thin body (UTB) SOI MOS-FETs [144], the application of bulk parameters is questionable.

In Section 2, the transport equations of the six moments model are given incorporating the extracted transport parameters for a 2D electron gas obtained by the Schrödinger-Poisson Solver VSP [145] self consistently coupled with the Subband Monte-Carlo simulator VMC [146]. The according extraction technique is presented in Section 3 followed by a discussion of the results in Section 4.

5.2 Transport Model

Higher-order transport models are systematically derived from Boltzmann's equation applying the method of moments [147]. Modeling the scattering operator by a macroscopic relaxation time approximation and multiplying with a proper set of weight functions, one obtains the drift-diffusion, the energy-transport and the six moments model [143]. The general moment equations read

$$\partial_t (nw_i) + \nabla \cdot (n\mathbf{V}_i) - i\mathbf{F} \cdot n\mathbf{V}_{i-1} = -n\frac{w_i - w_{i,0}}{\tau_i}, \quad (49)$$

$$n\mathbf{V}_{i} = -\frac{2\mu_{i}H_{i+1}}{3q} \left(\nabla(nw_{i+1}) - n\mathbf{F}w_{i}\frac{3+2iH_{i}}{2H_{i+1}}\right).$$
 (50)

In this hierarchy, the even moments describe conservation equations while the odd ones are fluxes. w_{i+1} are related to the average energies of each moment while \mathbf{V}_i is the average product of the velocity with the moment related energy. H_{i+1} are the non-parabolicity factors. Therefore the transport parameters arising in the six moment models are the carrier mobility μ_0 , the energy-flux mobility μ_1 , the energy relaxation time τ_1 , the second-order energy-flux mobility μ_2 , and the second-order energy relaxation time τ_2 .

5.3 Parameter Extraction

In order to efficiently and rigorously extract the required parameter set, a self consistent Schrödinger-Poisson Subband Monte Carlo (SP-SMC) simulator [145, 146] has been developed.

Based on the subband structure, MC calculations are performed taking phonon induced scattering and surface roughness scattering into account. The non-parabolicity of the band structure is treated by Kane's model. Parameters extracted at this step are valid within the low field regime. Once a driving field is applied in transport direction, the assumption of equilibrium carrier distribution is no longer valid: the carriers gain kinetic energy resulting in a reoccupation of the subband ladders (Fig. 43) which itself shifts the wavefunctions within the inversion layer. Hence, the scattering rates are affected following from the change in the overlap integral of the scattering operator. Furthermore, the subband ladder reconfiguration leads to a variation of the spatial distribution function of the electrons which itself has an impact on the shape of the potential well that forms the inversion channel (Fig. 44).



Figure 43: Populations of the first two subbands in the unprimed, primed, and double primed valleys versus the lateral field. Relative occupations are shifted to higher subbands in each valley for higher fields.

5.4 **Results**

As an example, a UTB structure with a film thickness of 5 nm and an acceptor doping of 2×10^{16} cm⁻³ has been investigated. After convergence of the SP-SMC loop is achieved, the parameters are extracted from the SMC simulator. The resulting carrier velocities as a function of the lateral field are presented in Figure 45. Due to different conduction masses in transport direction of each valley as well as a strong occupation of the primed valley in the high field regime (see Fig. 43), the total velocity is lower than in the unprimed and the double primed valley. In Figure 46, we show the mobilities in each valley and the total average mobility as a function of the channel thickness. To first order the mobilities are indirectly proportional to the effective masses. Therefore the difference of the mobilities are due to different conduction masses in each valley. The hump in the total average mobility is due to a high occupation of the unprimed ladder (see Fig.43). Increasing channel thickness results in an occupation of the remaining subband ladders. Hence the total mobility increases until the occupation of the other ladders reaches the same value. This is the maximum point, the hump.

A comparison of the energy-flux mobility and the kurtosis-flux mobility as well as the corresponding relaxation times between a 2D and bulk electron gas is



Figure 44: Conduction band and wavefunctions of a UTB SOI for different electric fields. Both the wavefunctions and subbands are shifted with increasing lateral fields.

shown in Figures 47 and 48, respectively. We observed that the higher-order mobilities of the 2D electron gas is higher than in the bulk case which can be explained as follows: Due to Heisenberg's uncertainty principle, there is a wider distribution of momentum in the quantization area, because of a higher localization of the particles than in the bulk. Hence there are more bulk phonons available that can assist the transition between electronic states. This will lead to an increase of the phonon rates and a decrease of the mobilities [148]. An increase of the phonon scattering rates will lead to a decrease of the relaxation times (see Fig. 48).

5.5 Conclusion

Advanced macroscopic transport models require an accurate set of transport parameters which are not directly accessible to measurements. With the presented approach it is possible to extract and tabulate a 2D parameter set for instance for the important case of ultra-thin body SOI MOSFETs.



Figure 45: Velocities in the first and second subband of the unprimed, primed, and double primed valleys as well as the average total velocity versus the lateral field. An effective field of 450 kV/cm is applied.



Figure 46: The mobilities of the unprimed, primed, and double primed valleys and the total average mobility as a function of the channel thickness at zero field condition.



0.6 $\overline{\underline{z}}_{\underline{\mu}}^{-} 0.4$ 0.2 0.2 0.4 0.2 0.6 0.8 0.60.

0.8

Figure 47: The energy-flux and the second-order energy flux mobility obtained by SP-SMC and bulk MC simulations. The mobilities behave analogously to the relaxation times.

Figure 48: A comparison of the subband MC results with the bulk case for the energy relaxation time and the second-order energy relaxation time. The increased scattering rates in the SMC case lead to lower relaxation times compared to the bulk case.

References

- R. H. Havemann and J. A. Hutchby. High-Performance Interconnects: An Integration Overview. *Proceedings of the IEEE*, 89(5):586 – 601, 2001.
- [2] S. Yokogawa, N. Okada, Y. Kakuhara, and H. Takizawa. Electromigration Performance of Multi-Level Damascene Copper Interconnects. *Microelectron. Reliab*, 41(9):1409–1416, 2001.
- [3] C.K. Hu and J.M.E. Harper. Copper Interconnections and Reliability. *Mater. Chem. Phys*, 52(5):5– 16, 1998.
- [4] L. Arnaud, T. Berger, and G. Reimbold. Evidence of Grain-Boundary Versus Interface Diffusion in Electromigration Experiments in Copper Damascene Interconnects. J. Appl. Phys., 93(1):192– 204, 2003.
- [5] M. A. Meyer, I. Zienert, and E. Zschech. Electron Backscatter Diffraction: Application to Cu Interconnects in Top-View and Cross Section. *Materials for Information Technology*, 1(1):95–100, 2005.
- [6] M. E. Sarychev and Yu. V. Zhitnikov. General Model for Mechanical Stress Evolution During Electromigration. J. Appl. Phys., 86(6):3068 – 3075, 1999.
- [7] H. Ye, C. Basaran, and D.C. Hopkins. Numerical Simulation of Stress Evolution During Electromigration in IC Interconnect Lines. *IEEE Trans. on Comp. and Pack.*, 26(3):673 – 681, 2003.
- [8] N.E. Meier, T.N. Marieb, P.A. Flinn, R.J. Gleixner, and J.C. Bravman. *In Situ* Studies of Electromigration Voiding in Passivated Copper Interconnects. *Proc. American Institute of Physics Conference*, 1999.
- [9] M. A. Meyer, M. Herrmann, E. Langer, and E. Zschech. In Situ SEM Observation of Electromigration Phenomena in Fully Embedded Copper Interconnect Structures. *Microelectronic Engineering*, 64:375–382, 2002.
- [10] M. A. Korhonen, P. Børgesen, K. N. Tu, and C.-Y. Li. Stress Evolution due to Electromigration in Confined Metal Lines. J. Appl. Phys., 73:3790, 1993.

- [11] G. L. Povirk. Numerical Simulations of Electromigration and Stress-Driven Diffusion in Polycrystalline Interconnects. *Proc. Mater. Res. Soc. Symp.*, 473:327–342, 1997.
- [12] S. Rzepka, M. A. Korhonen, E. R. Weber, and C. Y. Li. Three-Dimensional Finite Element Simulation of of Electro and Stress Migration Effects in Interconnect Lines. *Proc. Mater. Res. Soc. Symp.*, 473:329–335, 1997.
- [13] H. Ceric, R. Heinzl, Ch. Hollauer, T. Grasser, and S. Selberherr. Microstructure and Stress Aspects of Electromigration Modeling. *Stress-Induced Phenomena in Metallization, AIP*, 2006.
- [14] J. C. Fisher. Calculation of Diffusion Penetration Curves for Surface and Grain Boundary Diffusion. J. Appl. Phys., 22(1):74–77, 1951.
- [15] V. Sukharev. Simulation of Microstructure Influence on EM-Induced Degradation in Cu Interconnects. Stress-Induced Phenomena in Metallization: 8th International Workshop, AIP Conference Proceedings, this volume, 2005.
- [16] R. J. Gleixner, B. M. Clemens, and W. D. Nix. Void Nucleation in Passivated Interconnect Lines: Effects of Site Geometries, Interfaces, and Interface Flaws. *Journal of Materials Research*, 12:2081–2090, 1997.
- [17] D. R. Fridline and A. F. Bower. Influence of Anisotropic Surface Diffusivity on Electromigration Induced Void Migration and Evolution. J. Appl. Phys., 85(6):3168–3174, 1999.
- [18] M. Mahadevan and R. Bradley. Simulations and Theory of Electromigration-Induced Slit Formation in Unpassivated Single-Crystal Metal Lines. *Phys. Rev. B*, 59(16):11037–11046, 1999.
- [19] M. Mahadevan and R. Bradley. Phase Field Model of Surface Electromigration in Single-Crystal Metal Thin Films. *Physica D*, 126(3):201–213, 1999.
- [20] M. Mahadevan, R. Bradley, and J. M. Debierre. Simulation of an Electromigration-Induced Edge Instability in Single-Crystal Metal Lines. *Europhys. Lett.*, 45:680–685, 1999.
- [21] D. N. Bhate, A. Kummar, and A. F. Bower. Diffuse Interface Model for Electromigration and Stress Voiding. J. Appl. Phys., 87(4):1712–1721, 2000.

- [22] H. Ceric and S. Selberherr. An Adaptive Grid Approach for the Simulation of Electromigration Induced Void Migration. *IEICE Trans. Electronics*, (3):421–426, 2002.
- [23] J. Blowey and C. Elliott. The Chan-Hilliard Gradient Theory for Phase Separation with Non-Smooth Free Energy, Part II: Numerical Analysis. *European Journal of Applied Mathematics*, 3:147–179, 1992.
- [24] E. Baer, J. Lorenz, and H. Ryssel. Simulation of the Influence of Via Sidewall Tapering on Step Coverage of Sputter-Deposited Barrier Layers. *Microelectr. Eng.*, 64(1):321 – 328, 2002.
- [25] DEVISE User Manual, Release 10.0. Synopsys Switzerland Ltd., Switzerland, 2004.
- [26] E. Arzt, O. Kraft, W. D. Nix, and J. E. Sanchez. Electromigration Failure by Shape Change of Voids in Bamboo Lines. J. Appl. Phys., 76(3):1563–1571, 1994.
- [27] V. Huard, M. Denais, and C. Parthasarathy. NBTI Degradation: From Physical Mechanisms to Modelling. *Microelectr.Reliab.*, 46(1):1–23, 2006.
- [28] D.K. Schroder. Negative Bias Temperature Instability: What Do We Understand? *Microelectr.Reliab.*, 47(6):841–852, 2007.
- [29] S. Mahapatra, K. Ahmed, D. Varghese, A. E. Islam, G. Gupta, L. Madhav, D. Saha, and M. A. Alam. On the Physical Mechanism of NBTI in Silicon Oxynitride p-MOSFETs: Can Differences in Insulator Processing Conditions Resolve the Interface Trap Generation versus Hole Trapping Controversy? In *Proc. IRPS*, 2007.
- [30] T. Grasser. Negative Bias Temperature Instability: Modeling Challenges and Perspectives. In *Proc. IRPS*, 2008. (Tutorial).
- [31] B. Kaczer, V. Arkhipov, R. Degraeve, N. Collaert, G. Groeseneken, and M. Goodwin. Disorder-Controlled-Kinetics Model for Negative Bias Temperature Instability and its Experimental Verification. In *Proc. IRPS*, 2005.
- [32] C.R. Parthasarathy, M. Denais, V. Huard, G. Ribes, E. Vincent, and A.Bravaix. New Insights into Recovery Characteristics Post NBTI Stress. In *Proc. IRPS*, 2006.

- [33] C.R. Parthasarathy, M. Denais, V. Huard, C. Guerin, G. Ribes, E. Vincent, and A.Bravaix. Unified Perspective of NBTI and Hot-Carrier Degradation in CMOS using On-The-Fly Bias Patterns. In *Proc. IRPS*, 2007.
- [34] T. Grasser, B. Kaczer, Ph. Hehenberger, W. Goes, R. O'Connor, H. Reisinger, W. Gustin, and C. Schlünder. Simultaneous Extraction of Recoverable and Permanent Components Contributing to Bias-Temperature Instability. In *Proc. IEDM*, 2007.
- [35] K.O. Jeppson and C.M. Svensson. Negative Bias Stress of MOS Devices at High Electric Fields and Degradation of MNOS Devices. *J.Appl.Phys.*, 48(5):2004–2014, 1977.
- [36] S. Ogawa, M. Shimaya, and N. Shiono. Interface-Trap Generation at Ultrathin SiO₂ (4nm-6nm)-Si Interfaces During Negative-Bias Temperature Aging. J.Appl.Phys., 77(3):1137–1148, 1995.
- [37] M.A. Alam and S. Mahapatra. A Comprehensive Model of PMOS NBTI Degradation. *Microelectr.Reliab.*, 45(1):71–81, 2005.
- [38] T. Grasser, W. Goes, V. Sverdlov, and B. Kaczer. The Universality of NBTI Relaxation and its Implications for Modeling and Characterization. In *Proc. IRPS*, 2007.
- [39] M.A. Alam and H. Kufluoglu. On Quasi-Saturation of Negative Bias Temperature Degradation. *ECS Trans.*, 1(1):139–145, 2005.
- [40] A.T. Krishnan, C. Chancellor, S. Chakravarthi, P.E. Nicollian, V. Reddy, A. Varghese, R.B. Khamankar, and S. Krishnan. Material Dependence of Hydrogen Diffusion: Implications for NBTI Degradation. In *Proc. IEDM*, 2005.
- [41] H. Kufluoglu and M.A. Alam. A Generalized Reaction-Diffusion Model With Explicit H-H₂ Dynamics for Negative-Bias Temperature-Instability (NBTI) Degradation. *IEEE Trans.Electr.Dev.*, 54(5):1101–1107, 2007.
- [42] A.E. Islam, E. N. Kumar, H. Das, S. Purawat, V. Maheta, H. Aono, E. Murakami, S. Mahapatra, and M.A. Alam. Theory and Practice of Onthe-fly and Ultra-fast VT Measurements for NBTI Degradation: Challenges and Opportunities. In *Proc. IEDM*, 2007.
- [43] S. Rangan, N. Mielke, and E.C.C. Yeh. Universal Recovery Behavior of Negative Bias Temperature Instability. In *Proc. IEDM*, 2003.

- [44] D.S. Ang, S. Wang, and C.H. Ling. Evidence of Two Distinct Degradation Mechanisms from Temperature Dependence of Negative Bias Stressing of the Ultrathin Gate p-MOSFET. *IEEE Electron Device Lett.*, 26(12):906–908, 2005.
- [45] C. Shen, M.-F. Li, C. E. Foo, T. Yang, D.M. Huang, A. Yap, G.S. Samudra, and Y.-C. Yeo. Characterization and Physical Origin of Fast V_{th} Transient in NBTI of pMOSFETs with SiON Dielectric. In *Proc. IEDM*, 2006.
- [46] A. Haggag, G. Anderson, S. Parihar, D. Burnett, G. Abeln, J. Higman, and M. Moosa. Understanding SRAM High-Temperature-Operating-Life NBTI: Statistics and Permanent vs Recoverable Damage. In *Proc. IRPS*, 2007.
- [47] V. Huard, C. Parthasarathy, N. Rallet, C. Guerin, M. Mammase, D. Barge, and C. Ouvrard. New Characterization and Modeling Approach for NBTI Degradation from Transistor to Product Level. In *Proc. IEDM*, 2007.
- [48] M. Denais, A. Bravaix, V. Huard, C. Parthasarathy, C. Guerin, G. Ribes, F. Perrier, M. Mairy, and D. Roy. Paradigm Shift for NBTI Characterization in Ultra-Scaled CMOS Technologies. In *Proc. IRPS*, 2006.
- [49] T.L. Tewksbury and H.-S. Lee. Characterization, Modeling, and Minimization of Transient Threshold Voltage Shifts in MOSFETs. *IEEE J.Solid-State Circuits*, 29(3):239–252, 1994.
- [50] V. Reddy, A.T. Krishnan, A. Marshall, J. Rodriguez, S. Natarajan, T. Rost, and S. Krishnan. Impact of Negative Bias Temperature Instability on Digital Circuit Reliability. In *Proc. IRPS*, 2002.
- [51] D.K. Schroder and J.A. Babcock. Negative Bias Temperature Instability: Road to Cross in Deep Submicron Silicon Semiconductor Manufacturing. *J.Appl.Phys.*, 94(1):1–18, 2003.
- [52] J.P. Campbell, P.M. Lenahan, C.J. Cochrane, A.T. Krishnan, and S. Krishnan. Atomic-Scale Defects Involved in the Negative-Bias Temperature Instability. *IEEE Trans.Dev.Mat.Rel.*, 7(4):540–557, 2007.
- [53] H. Reisinger, U. Brunner, W. Heinrigs, W. Gustin, and C. Schlünder. A Comparison of Fast Methods for Measuring NBTI Degradation. *IEEE Trans.Dev.Mat.Rel.*, 7(4):531–539, 2007.
- [54] A.K. Jonscher and S. Bozdemir. All Forms of Relaxation Take Place in Fractal Time. *IEEE EIM*, 11(2):30–33, 1995.

- [55] W. Kauzmann. Dielectric Relaxation as a Chemical Rate Process. *Rev.Mod.Phys*, 14(1):12–44, 1942.
- [56] J.R. Jameson, W. Harrison, P.B. Griffin, J.D. Plummer, and Y. Nishi. A Semiclassical Model of Dielectric Relaxation in Glasses. *J.Appl.Phys.*, 100(1):124101, 2006.
- [57] W.A. Phillips. Tunneling States in Amorphous Solids. J.Low.Temp.Phys, 7(3/4):351–360, 1972.
- [58] P.W. Anderson, B.I. Halperin, and C.M. Varma. Anomalous Low-temperature Thermal Properties of Glasses and Spin Glasses. *Philos.Mag.*, 25:1–9, 1972.
- [59] B. Tuttle and C.G. Van de Walle. Structure, Energetics, and Vibrational Properties of Si-H Bond Dissociation in Silicon. *Phys.Rev.B*, 59(20):12884–12889, 1999.
- [60] R. Biswas, Y.-P. Li, and B.C. Pan. Enhanced Stability of Deuterium in Silicon. *Appl.Phys.Lett.*, 72(26):3500–3502, 1998.
- [61] A. Stesmans. Passivation of P_{b0} and P_{b1} Interface Defects in Thermal (100) Si/SiO₂ with Molecular Hydrogen. *Appl.Phys.Lett.*, 68(15):2076–2078, 1996.
- [62] A. Stesmans. Dissociation Kinetics of Hydrogen-Passivated P_b Defects at the (111)Si/SiO₂ Interface. *Phys.Rev.B*, 61(12):8393–8403, 2000.
- [63] L.-A. Ragnarsson and P. Lundgren. Electrical Characterization of P_b Centers in (100)Si/SiO₂ Structures: The Influence of Surface Potential on Passivation During Post Metallization Anneal. *J.Appl.Phys.*, 88(2):938–942, 2000.
- [64] J.P. Campbell, P.M. Lenahan, A.T. Krishnan, and S. Krishnan. Direct Observation of the Structure of Defect Centers Involved in the Negative Bias Temperature Instability. *Appl.Phys.Lett.*, 87(20):1–3, 2005.
- [65] W.B. Jackson. Role of Band-Tail Carriers in Metastable Defect Formation and Annealing in Hydrogenated Amorphous Silicon. *Phys.Rev.B*, 41(2):1059–1075, 1990.
- [66] S. Zafar. Statistical Mechanics Based Model for Negative Bias Temperature Instability Induced Degradation. J.Appl.Phys., 97(10):1–9, 2005.

- [67] M. Houssa, M. Aoulaiche, S. De Gendt, G. Groeseneken, M.M. Heyns, and A. Stesmans. Reaction-Dispersive Proton Transport Model for Negative Bias Temperature Instabilities. *Appl.Phys.Lett.*, 86(9):1–3, 2005.
- [68] T. Grasser, W. Goes, and B. Kaczer. Dispersive Transport and Negative Bias Temperature Instability: Boundary Conditions, Initial Conditions, and Transport Models. *IEEE Trans.Dev.Mat.Rel.*, 8(1):79–97, 2008.
- [69] A. Haggag, W. McMahon, K. Hess, K. Cheng, J. Lee, and J. Lyding. High-Performance Chip Reliability from Short-Time-Tests. In *Proc. IRPS*, 2001.
- [70] L. Tsetseris, X.J. Zhou, D.M. Fleetwood, R.D. Schrimpf, and S.T. Pantelides. Physical Mechanisms of Negative-Bias Temperature Instability. *Appl.Phys.Lett.*, 86(14):1–3, 2005.
- [71] J.W. McPherson. Quantum Mechanical Treatment of Si-O Bond Breakage in Silica Under Time Dependent Dielectric Breakdown Testing. In *Proc. IRPS*, 2007.
- [72] T. Grasser, P.-J. Wagner, Ph. Hehenberger, W. Goes, and B. Kaczer. A Rigorous Study of Measurement Techniques for Negative Bias Temperature Instability. In *IIRW Final Rep.*, 2007.
- [73] B. Kaczer, V. Arkhipov, R. Degraeve, N. Collaert, G. Groeseneken, and M. Goodwin. Temperature Dependence of the Negative Bias Temperature Instability in the Framework of Dispersive Transport. *Appl.Phys.Lett.*, 86(14):1–3, 2005.
- [74] R. Fernandez, B. Kaczer, A. Nackaerts, S. Demuynck, R. Rodriguez, M. Nafria, and G. Groeseneken. AC NBTI Studied in the 1 Hz - 2 GHz Range on Dedicated On-Chip CMOS Circuits. In *Proc. IEDM*, 2006.
- [75] K. Kang, H. Kufluoglu, K. Roy, and M. Ashraful Alam. Impact of Negative-Bias Temperature Instability in Nanoscale SRAM Array: Modeling and Analysis. *IEEE Trans.Computer-Aided Design*, 26(10):1770–1781, 2007.
- [76] M.A. Alam. A Critical Examination of the Mechanics of Dynamic NBTI for PMOSFETs. In *Proc. IEDM*, 2003.
- [77] S. Chakravarthi, A.T. Krishnan, V. Reddy, C.F. Machala, and S. Krishnan. A Comprehensive Framework for Predictive Modeling of Negative Bias Temperature Instability. In *Proc. IRPS*, 2004.

- [78] B. Kaczer, T. Grasser, Ph.J. Roussel, J. Martin-Martinez, R. O'Connor, B.J. O'Sullivan, and G. Groeseneken. Ubiquitous Relaxation in BTI Stressing-New Evaluation and Insights. In *Proc. IRPS*, 2008.
- [79] J. R. Black. Electromigration-A Brief Survey and Some Recent Results. *IEEE Trans. Elec. Dev.*, 16(4):338–347, 1969.
- [80] R. Rosenberg and M. Ohring. Void Formation and Growth During Electromigration in Thin Films. J. Appl. Phys., 47:5671, 1971.
- [81] I. A. Blech and C. Herring. Stress Generation by Electromigration. J. Appl. Phys., 29(3):131–133, 1976.
- [82] I. A. Blech. Electromigration in Thin Aluminum Films on Titanium Nitride. J. Appl. Phys., 47(4):1203–1208, 1976.
- [83] I. A. Blech and K. L. Tai. Measurement of Stress Gradients Generated by Electromigration. *Appl. Phys. Lett*, 30(8):387–389, 1976.
- [84] R. Kirchheim. Stress and Electromigration in Al-Lines of Integrated Circuits. *Acta Metallurg. Mater.*, 40(2):309–323, 1992.
- [85] J.R. Lloyd and E. Arzt. A Simple Model for Stress Voiding in Passivated Thin Film Conductors. Symposium Proc. on Materials Reliability in Microelectronics II, 265:45–57, 1992.
- [86] J.R. Lloyd and J.J.Clement. Electromigration in Copper Conductors. *Thin Solid Films*, 262(1):135–141, 1995.
- [87] J. J. Clement. Electromigration Modeling for Integrated Circuit Interconnect Reliability Analysis. *IEEE Trans. on Dev. and Mat. Rel.*, 1(1):33–42, 2001.
- [88] M. E. Sarychev, Yu. V. Zhitnikov, L. Borucki, C. L. Liu, and T. M. Makhviladze. General Model for Mechanical Stress Evolution During Electromigration. J. Appl. Phys., 86(6):3068– 3075, 1999.
- [89] S.H. Rhee, Y. Du, and P. S. Ho. Thermal Stress Characteristics of Cu/Oxide and Cu/low-k Submicron Interconnect Structures. J. Appl. Phys., 2003.
- [90] J. R. Lloyd. Electromigration in thin film conductors. Semicond. Sci. Technol., 12:1177, 1997.
- [91] P. H. Dederichs and K. Schroeder. Anisotropic Diffusion in Stress Fields. *Phys. Rev. B*, 17:2524, 1978.

- [92] M. Diebel and S. T. Dunham. Ab-initio Calculations to Predict Stress Effects on Defects and Diffusion in Silicon. In Proc. of Simulation of Semiconductor Process and Devices (SISPAD), volume 147, 2003.
- [93] H. Ceric, C. H. Hollauer, and S. Selberherr. Simulation of Texture Development Caused Stress Build-Up in Electroplated Copper Lines. In Proc. of 13th Internation Symposium on the Physical and Failure Analysis of Integrated Circuits (IPFA), volume 359, Singapore, 2006.
- [94] H. Ceric. Numerical Techniques in Modern TCAD. Dissertation, Institute for Microelectronics, Vienna University of Technology, 2005.
- [95] International Technology Roadmap for Semiconductors. Technical report, Semiconductor Industry Association, 2007.
- [96] R. Saito, T. Takeya, T. Kimura, G. Dresselhaus, and M. S. Dresselhaus. Raman Intensity of Single-Wall Carbon Nanotubes. *Phys. Rev. B*, 57(7):4145–4153, 1998.
- [97] R. Martel, T. Schmidt, H. Shea, T. Hertel, and P. Avouris. Single- and Multi-Wall Carbon Nanotube Field-Effect Transistors. *Appl. Phys. Lett.*, 73(17):2447–2449, 1998.
- [98] W. Hoenlein, F. Kreupl, G. Duesberg, A. Graham, M. Liebau, R. Seidel, and E. Unger. Carbon Nanotube Applications in Microelectronics. *IEEE Trans. Comp. Packag. Technol.*, 27(4):629– 634, 2004.
- [99] J. Appenzeller. Carbon Nanotubes for High-Performance Electronics–Progress and Prospects. In *Proc. IEEE*, volume 96. Proc. IEEE, 2008.
- [100] P. Avouris, Z. Chen, and V. Perebeinos. Carbon Based Electronics. *Nature Nanotechnology*, 2(10):605–615, 2007.
- [101] A. Javey, J. Guo, Q. Wang, M. Lundstrom, and H. Dai. Ballistic Carbon *Nature (London)*, 424(6949):654–657, 2003.
- [102] R. V. Seidel, A. P. Graham, J. Kretz, B. Rajasekharan, G. S. Duesberg, M. Liebau, E. Unger, F. Kreupl, and W. Hoenlein. Sub-20 nm Short Channel Carbon Nanotube Transistors. *Nano Lett.*, 5(1):147–150, 2005.
- [103] J.-Y. Park. Carbon Nanotube Field-Effect Transistor with a Carbon Nanotube Gate Electrode. *Nanotechnology*, 18(9):0952002, 2007.

- [104] R. Saito, G. Dresselhaus, and M. Dresselhaus. *Physical Properties of Carbon Nanotubes*. London: Imperial College Press, 1998.
- [105] M. Freitag, J. Chen, J. Tersoff, J. Tsang, Q. Fu, J. Liu, and P. Avouris. Mobile Ambipolar Domain in Carbon-Nanotube Infrared Emitters. *Phys. Rev. Lett.*, 93:076803, 2004.
- [106] M. Freitag, Y. Martin, J. Misewich, R. Martel, and P. Avouris. Photoconductivity of Single Carbon Nanotubes. *Nano Lett.*, 3(9):1067–1071, 2003.
- [107] A. Svizhenko, M. P. Anantram, T. R. Govindan, B. Biegel, and R. Venugopal. Two-Dimensional Quantum Mechanical Modeling of Nanotransistors. J. Appl. Phys., 91(4):2343–2354, 2002.
- [108] A. Svizhenko and M. P. Anantram. Role of Scattering in Nanotransistors. *IEEE Trans. Electron Devices*, 50(6):1459–1466, 2003.
- [109] R. Venugopal, M. Paulsson, S. Goasguen, S. Datta, and M. S. Lundstrom. A Simple Quantum Mechanical Treatment of Scattering in Nanoscale Transistors. J. Appl. Phys., 93(9):5613–5625, 2003.
- [110] M. B. Nardelli. Electronic Transport in Extended Systems: Application to Carbon Nanotubes. *Phys. Rev. B*, 60(11):7828–7833, 1999.
- [111] J. Taylor, H. Guo, and J. Wang. Ab Initio Modeling of Quantum Transport Properties of Molecular Electronic Devices. *Phys. Rev. B*, 63:245407, 2001.
- [112] J. J. Palacios, A. J. P. Jimenez, E. Louis, E. San-Fabioa, and J. Verges. First-Principles Phase-Coherent Transport in Metallic Nanotubes with Realistic Contacts. *Phys. Rev. Lett.*, 90:106801, 2003.
- [113] Y. Xue and M. A. Ratner. Schottky Barriers at Metal-Finite Semiconducting Carbon Nanotube Interfaces. *Appl. Phys. Lett.*, 83(12):2429–2431, 2003.
- [114] J. Guo. A Quantum-Mechanical Treatment of Phonon Scattering in Carbon Nanotube Transistors. J. Appl. Phys., 98:063519, 2005.
- [115] J. Guo, S. Hassan, A. Javey, G. Bosman, and M. Lundstrom. Assessment of High-Frequency Performance Potential of Carbon Nanotube Transistors. *IEEE Trans. Nanotechnol.*, 4(6):715–721, 2005.

- [116] A. Svizhenko, M. P. Anantram, and T. R. Govindan. Ballistic Transport and Electrostatics in Metallic Carbon Nanotubes. *IEEE Trans. Nanotechnol.*, 4(5):557–562, 2005.
- [117] A. Svizhenko and M. Anantram. Effect of Scattering and Contacts on Current and Electrostatics in Carbon Nanotubes. *Phys. Rev. B*, 72:085430, 2005.
- [118] M. Pourfath and H. Kosina. The Effect of Phonon Scattering on the Switching Response of Carbon Nanotube FETs. *Nanotechnology*, 18:424036–6, 2007.
- [119] W. Tian, S. Datta, S. Hong, R. Reifenberger, J. I. Henderson, and C. P. Kubiak. Conductance Spectra of Molecular Wires. J. Chem. Phys, 109(7):2874–2882, 1998.
- [120] P. S. Damle, A. W. Ghosh, and S. Datta. Unified Description of Molecular Conduction: From Molecules to Metallic Wires. *Phys. Rev. B*, 64:201403, 2001.
- [121] J. M. Seminario, L. E. Cordova, and P. A. Derosa. An Ab Initio Approach to the Calculation of Current-Voltage Characteristics of Programmable Molecular Devices. *Proc. IEEE*, 91(11):1958– 1975, 2003.
- [122] M. Galperin, A. Nitzan, S. Sek, and M. Majda. Asymmetric Electron Transmission across Asymmetric Alkanethiol Bilayer Junctions. J. Electroanal. Chem., 550-551(1):337–350, 2003.
- [123] Y. Xue and M. A. Ratner. End Group Effect on Electrical Transport through Individual Molecules: A Microscopic Study. *Phys. Rev. B*, 69:085403, 2004.
- [124] A. W. Ghosh, T. Rakshit, and S. Datta. Gating of a Molecular Transistor: Electrostatic and Conformational. *Nano Lett.*, 4(4):565–568, 2004.
- [125] G. D. Mahan. *Many-Particle Physics*. ser. Physics of Solids and Liquids. Plenum Press, New York, 2nd edition, 1990.
- [126] S. Datta. Electronic Transport in Mesoscopic Systems. Cambridge University Press, New York, 1995.
- [127] J. Guo, S. Datta, M. Lundstrom, and M. Anantram. Multi-Scale Modeling of Carbon Nanotube Transistors. *The International Journal of Multiscale Computational Engineering*, 2(2):257–278, 2004.

- [128] R. Venugopal, Z. Ren, S. Datta, M. Lundstrom, and D. Jovanovic. Simulating Quantum Transport in Nanoscale Transistors: Real Versus Mode-Space Approaches. J. Appl. Phys., 92(7):3730– 3739, 2002.
- [129] V. N. Popov and P. Lambin. Intraband Electron-Phonon Scattering in Single-Walled Carbon Nanotubes. *Phys. Rev. B*, 74:075415, 2006.
- [130] R. Lake and S. Datta. Nonequilibrium Green's-Function Method Applied to Double-Barrier Resonant-Tunneling Diodes. *Phys. Rev. B*, 45(12):6670–6685, 1992.
- [131] M. Pourfath and H. Kosina. A Fast and Stable Poisson-Schrödinger Solver for the Analysis of Carbon Nanotube Transistors. J. Comp. Electronics, 5(2):155–159, 2006.
- [132] S. O. Koswatta, S. Hasan, M. Lundstrom, M. P. Anantram, and D. E. Nikonov. Ballisticity of Nanotube FETs: Role of Phonon Energy and Gate Bias. *Appl. Phys. Lett.*, 89:023125, 2006.
- [133] Y. Yoon, Y. Ouyang, and J. Guo. Effect of Phonon Scattering on Intrinsic Delay and Cutoff Frequency of Carbon Nanotube FETs. *IEEE Trans. Electron Devices*, 53(10):2467–2470, 2006.
- [134] Y. Chen, Y. Ouyang, J. Guo, and T. X. Wu. Time-Dependent Quantum Transport and Nonquasistatic Effects in Carbon Nanotube Transistors. *Appl. Phys. Lett.*, 89:203122, 2006.
- [135] M. Lundstrom. Elementary Scattering Theory of the Si MOSFET. *IEEE Electron Device Lett.*, 18(7):361–363, 1997.
- [136] A. Javey, J. Guo, D. Farmer, Q. Wang, E. Yenilmez, R. Gordon, M. Lundstrom, and H. Dai. Self-Aligned Ballistic Molecular Transistors and Electrically Parallel Nanotube Arrays. *Nano Lett.*, 4(7):1319–1322, 2004.
- [137] J. Park, S. Rosenblatt, Y. Yaish, V. Sazonova, H. Ustunel, S. Braig, T. Arias, P. Brouwer, and P. McEuen. Electron-Phonon Scattering in Metallic Single-Walled Carbon Nanotubes. *Nano Lett.*, 4(3):517–520, 2004.
- [138] D. Singh, K. Jenkins, J. Appenzeller, D. Neumayer, A. Grill, and H.-S. P. Wong. Frequency Response of Top-Gated Carbon Nanotube Field-Effect Transistors. *IEEE Trans. Nanotechnol.*, 3(3):383–387, 2004.

- [139] D. Frank and J. Appenzeller. High-Frequency Response in Carbon Nanotube Field-Effect Transistors. *IEEE Electron Device Lett.*, 25(1):34–36, 2004.
- [140] X. Huo, M. Zhang, P. C. H. Chan, Q. Liang, and Z. K. Tang. High Frequency S parameters Characterization of Back-Gate Carbon Nanotube Field-Effect Transistors. San Francisco: IEEE Intl. Electron Device Meet. Tech. Dig., 2004.
- [141] A. L. Louarn, F. Kapche, J.-M. Bethoux, H. Happy, G. Dambrine, V. Derycke, P. Chenevier, N. Izard, M. F. Goffman, and J. Bourgoin. Intrinsic Current Gain Cutoff Frequency of 30 GHz with Carbon Nanotube Transistors. *Appl. Phys. Lett.*, 90:233108, 2007.
- [142] T. Grasser, C. Jungemann, H. Kosina, B. Meinerzhagen, and S. Selberherr. Advanced Transport Models for Sub-Micrometer Devices. In *Proc. SISPAD*, Munich, Germany, 2004.
- [143] T. Grasser, R. Kosik, C. Jungemann, H. Kosina, and S. Selberherr. Non-Parabolic Macroscopic Transport Models for Device Simulation Based on Bulk Monte Carlo Data. J.Appl.Phys., 97(9):1–12, 2005.

- [144] H. Lucci, D. Esseni, P. Palestri, and L. Selmi. Comparative Analysis of Basic Transport Properties in the Inversion Layer of Bulk and SOI MOS-FETs: a Monte-Carlo Study. In *Proc. ESSDERC*, 2004.
- [145] M. Karner, A. Gehring, S. Holzer, M. Pourfath, M. Wagner, H. Kosina, T. Grasser, and S. Selberherr. VSP - A Multi-Purpose Schrödinger-Poisson Solver for TCAD Applications. In *11th IWCE*, 2006.
- [146] http://www.iue.tuwien.ac.at/software. VMC 2.0 User's Guide. Institut für Mikroelektronik, Technische Universität Wien, Austria, 2006.
- [147] T. Grasser. Non-Parabolic Macroscopic Transport Models for Semiconductor Device Simulation. *Physica A*, 349(1/2):221–258, 2005.
- [148] F. Gamiz and M. V. Fischetti. Monte Carlo Simulation of Double-Gate Silicon-On Insulator Inversion Layers: The Role of Volume Inversion. J. Appl. Phys, 89(10):5478–5486, 2001.