

Negative bias temperature instability modeling for high-voltage oxides at different stress temperatures

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Available online 1 March 2007

Abstract

The temperature bias instability of high-voltage oxides is analyzed. For the investigation of negative bias temperature instability (NBTI) we present an enhanced reaction–diffusion model including trap-controlled transport, the amphoteric nature of the P_b centers at the Si/SiO₂ interface, Fermi-level dependent interface charges, and fully self-consistent coupling to the semiconductor device equations. Comparison to measurement data for a stress/relaxation cycle and a wide range of temperatures shows excellent agreement.

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1. Introduction

Negative bias temperature instability (NBTI) has come to the forefront of scientific interest. It occurs in p-type MOS devices stressed with negative gate bias at elevated temperatures. In particular for thicker oxides, as used in high-voltage devices, evidence has been found that the degradation is dependent on two major effects, the generation of interface-traps N_{it} at the Si/SiO₂ interface and the transport of a mobile, hydrogen related species into the dielectric. The generation of interface-traps leads to a shift of important transistor parameters such as the threshold voltage V_{th} , the drain current I_d , the transconductance g_m , and the off current I_{off} . Due to the need for accurate prediction of device and circuit lifetimes, modeling and simulation of the degradation physics has gained importance. There are two important factors for accurate modeling: (a) the physics of the degradation mechanisms have to be modeled as precisely as possible (b) the experimental and measurement setup must lead to an exact description of the device state.

Here, especially the applied measurement technique needs special attention, as the method used for evaluating NBTI degradation can have a considerable impact on lifetime extrapolation results [1,2].

2. The reaction–diffusion model

The original reaction–diffusion (RD) model was proposed by Jeppson and Svensson thirty years ago [3]. Since then the model has been continuously refined. It describes the degradation process as a reaction at the Si/SiO₂ interface generating an interface state, N_{it} , as well as releasing a mobile hydrogen related species, N_X . This generation process is described as

$$\frac{\partial N_{it}(t)}{\partial t} = \underbrace{k_f(N_0 - N_{it}(t))}_{\text{generation}} - \underbrace{k_r N_{it}(t) N_X(0, t)^{1/a}}_{\text{annealing}}. \quad (1)$$

where k_f is the interface-trap generation and k_r the annealing rate. The symbol N_0 denotes the initial number of electrically inactive Si–H bonds and $N_X(0, t)$ is the surface concentration of the diffusing species. The value of a gives the order of the reaction. Originally, neutral hydrogen, H^0 , was proposed which is obtained with $a = 1$. For molecular

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hydrogen, H_2 , $a = 2$ where the molecule is assumed to be formed in the vicinity of the interface.



The equilibrium of the forward and backward reaction is controlled by the hydrogen density at the interface $N_X(0, t)$. Thus, the transport mechanism of the hydrogen species away from the interface characterizes the degradation mechanism, controlling for example the V_{th} shift. The original reaction–diffusion model describes the transport as a purely diffusive mechanism which is expressed by the regular diffusion equation

$$\frac{\partial N_X(x, t)}{\partial t} = D \nabla^2 N_X(x, t). \quad (3)$$

Here D is the diffusivity of the hydrogen species in the dielectric. As boundary condition for the Si/SiO₂ interface the influx of the newly created species has to be considered as $\partial N_{it}/\partial t/a$.

3. Dispersive hydrogen transport

Instead of using the standard diffusion equation [3,4] we assume trap-controlled, dispersive transport of the hydrogen species [1]. The species N_X consists of conducting, N_c , and trapped, N_t , particles. The trapped particles are distributed in energy, where the density at a trap energy-level E_t is given as $\rho(\mathbf{x}, E_t, t)$. The trapped particles do not contribute to the transport. Thus, (3) transforms to

$$\frac{\partial N_c(\mathbf{x}, t)}{\partial t} + \frac{\partial N_t(\mathbf{x}, t)}{\partial t} = D \nabla^2 N_c(\mathbf{x}, t). \quad (4)$$

At each trap energy-level a rate equation describes the dynamics between trapping and de-trapping as

$$\frac{\partial \rho(E_t)}{\partial t} = c(E_t) N_c(g(E_t) - \rho(E_t)) - r(E_t) \rho(E_t). \quad (5)$$

Here $c(E_t)$ and $r(E_t)$ are the energy-dependent capture and release rates, and $g(E_t)$ is the trap density-of-states (DOS), where commonly an exponential distribution is assumed.

4. TCAD simulation

The reaction–diffusion model has been implemented in a two- and three-dimensional numerical device simulator [5] and the model equations are coupled fully self-consistently to the semiconductor device equations. The benefits are manifold, since now the local oxide field, hole concentration, charged carriers, and fast interface states (Fermi-level dependent charges) can be included in both the device equations and the NBTI model. Due to the availability of the solution of the semiconductor equations, the trap generation rate can be expressed as a function of the surface hole concentration p_s and the oxide electric field E_{ox} as $k_f = k_{f,0} p_s/p_{ref} \exp(E_{ox}/E_{ref})$ [6] instead of using estimates for p and a constant E_{ox} . The symbols $k_{f,0}$, p_{ref} , and E_{ref}

denote the reference values for the generation rate, the hole concentration and the electric field.

The amphoteric nature of the P_b centers at the Si/SiO₂ interface, which form the interface-traps N_{it} , is considered. The DOS of the P_b centers in the Si bandgap forms two distinct peaks of Gaussian shape [7]. P_b centers in the upper peak are assumed acceptor-like. They are electrically neutral when the Fermi-level is below the trap, and negatively charged otherwise. The traps in the lower peak are donor-like, neutral when the Fermi-level is energetically above and positively charged otherwise. The consideration of the exact DOS is important when the Fermi-level is not close to the valence band, as in measurement cycles.

For the comparison of measurements to simulation results the complete dynamics of degradation and annealing during the measurement intervals have to be taken into account. In our simulations we mimic the whole measurement procedure as closely as possible to reflect the real world conditions and to reduce the error due to the measurement delays.

5. Experiment and results

The device under test was a 48 nm high-voltage oxide stressed for 1000 s at $V_g = -25$ V at four different temperatures (100, 125, 150, and 175 °C). A 1000 s relaxation phase with $V_g = 0$ V followed the stress phase. To determine the threshold voltage shift ΔV_{th} , the stress was interrupted for 2 s at each measurement point to perform a gate voltage sweep from 0 V to -2 V. During this period a remarkable amount of relaxation can be observed. Thus, it is crucial to include the recovery process in the model. The important advantage is that the threshold voltage can now be extracted from the simulation results in the same way as in the measurements. In contrast to the

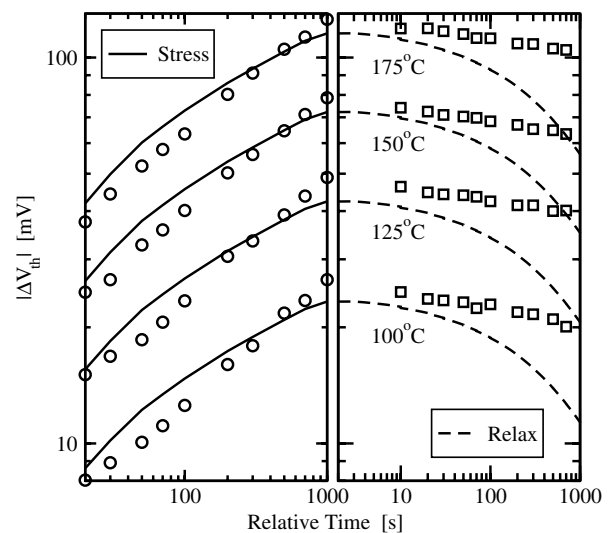


Fig. 1. Comparison of the measurements to simulation results using the standard reaction–diffusion model. The model fails to reproduce measurement data, especially in the relaxation phase.

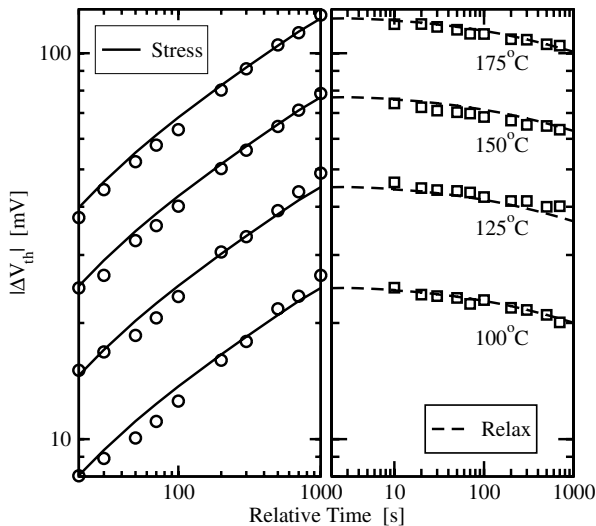


Fig. 2. Comparison of the measurements to simulation results using the extended model. The slope of $n = 0.31$ during the stress phase is very well matched with the trap-controlled transport model and the agreement in the relaxation phase is excellent.

standard reaction–diffusion model (Fig. 1), the extended model (Fig. 2) shows excellent agreement with measurement data for a wide range of temperatures, which can be achieved using a single set of model parameters. During the faster process within the first few seconds the annealing is attributed to re-passivation of dangling Si/SiO₂ interface bonds with hydrogen from shallow traps close to the interface. After the consumption of all quickly available hydrogen, additional hydrogen can only be provided by de-trapping from deep traps in the oxide bulk, which is a slower process. As the transition is seamless, there is no change in the time exponent during annealing. To properly capture the relaxation phase, the DOS used in the dispersive transport equation is modeled by an exponential tail for shallow traps for fast trapping and de-trapping, while the slow process is governed by deep traps given by an additional Gaussian peak well below the hydrogen conduction band.

6. Conclusion

We have presented an enhanced NBTI reaction–diffusion model with dispersive transport and fully self-consistent coupling to the semiconductor device equations. The amphoteric nature of the P_b centers and its Fermi-level dependent charge state is modeled. The implementation of the model in a multi-dimensional numerical device simulator allows us to directly use many commonly approximated quantities such as the oxide electric field or the interface hole concentration in a self-consistent manner. The model has been calibrated to measurement data of a high-voltage MOSFET structure at a wide range of temperatures for both, a stress and a relaxation cycle. Here the full measurement setup has been taken into account and very good agreement has been shown. To extend the model from thick SiO₂ dielectrics to thin, nitrided oxides of state-of-the-art logic MOSFETs it might be necessary to include additional effects such as hole trapping.

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