Defect creation kinetics in amorphous silicon thin film transistors

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Abstract

The rate of defect creation in amorphous silicon thin film transistors, under gate bias stress, is proportional to $N_{BT}^a B t^b / C_0^{1/2}$, where $N_{BT}$ is the bandtail carrier density. Experimentally $a$ is 1.5–1.9, while $b$ is 0.5–0.6. We have developed a model to account for this dependence, based on an exponential distribution of barriers to defect creation. The key new feature of our model is that we include the backward reaction, as well as the forward reaction, and also the effect of the charge-state of the formed defects. Considering the forward reaction only, leads to $a = b$, while a full analysis leads to the simple new result that $a / C^{25} = 3 b$, which is in excellent agreement with experiments.

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1. Introduction

A few years after the first demonstration of the field effect in amorphous silicon [1], the instability of the threshold voltage was observed [2]. It was first assumed that charge injection into the silicon nitride gate insulator is the dominant mechanism for the threshold voltage shift [2]. However, it turned out that additional defect state creation dominates for moderate bias in high-quality TFTs [3].

There are many empirical models in the literature, which attempt to model the threshold voltage shift $\Delta V_t$ in TFTs. These are sometimes based on charge trapping in the insulator [2,4], sometimes on defect state creation [3,5–7] or sometimes are simply descriptive [8]. A commonly used formula is the stretched exponential, first proposed by Jackson and Moyer in 1987 [5]

$$\Delta V_t(t) = V_0 \left[ 1 - \exp \left( - (t/t_0)^\beta \right) \right]$$

with $V_0$ the gate bias over the initial threshold $V_g - V_t$, $t_0 = v_e^{-1} \exp(E_A/kT)$ where $E_A$ is an activation energy and $v_e$ an attempt-to-escape frequency and $\beta = T/T_0$.

In the following, we consider only moderate bias where state creation is dominant. Then, the threshold voltage shift $\Delta V_t$ is proportional to the number of created defects $\Delta N_D(t)$ in a TFT under gate bias stress due to the capacitor.
configuration $C\Delta V_i = \Delta N_D$ with $C$ the capacitance of the TFT.

Several groups have observed a significant deviation from a stretched exponential time dependence \([4,6–8]\). In particular, the dependence of the defect creation rate $dN_D(t)/dt$ on the number of band tail carriers $N_{BT}$ was not correctly described by Eq. (1). Recently, we have presented an improved, semi-empirical kinetic equation for defect creation \([6]\).

$$\frac{dN_D(t)}{dt} = - \frac{dN_{BT}(t)}{dt} = kN_{BT}(t)^{\alpha} \frac{t^{\beta-1}}{t_0^{\beta}}$$  \(2\)

with $\alpha = 1.5–1.9$, $k = \text{const}$ and $t_0 = v_c^{-1} \exp(E_A/kT)$, where $E_A$ is related to the most probable energy barrier for defect creation and $v_c$ the attempt-to-escape frequency for defect creation. An analytic solution is possible for $1 < \alpha < 2$ which yields a ’stretched hyperbola’ of the form

$$\Delta N_D(t) = N_{BT}^0 \left\{ 1 - \frac{1}{\left[ 1 + (t/t_0)^{\beta} \right]^{1/\alpha}} \right\}$$  \(3\)

with $\varepsilon = \alpha - 1$ and $N_{BT}^0$ the initial density of bandtail carriers. We have shown \([6]\) that this stretched hyperbola fit is an improvement compared to the commonly used stretched exponential fit ($\alpha = 1$), since Eq. (2) takes into account the super-linear bias dependence $N_{BT}^\alpha$. Note that Jackson \([7]\) already proposed a similar kind of equation in 1990 based on a modified hydrogen diffusion concept involving a carrier-dependent hydrogen diffusion constant.

Up to now, all models are completely empirical or semi-empirical by incorporating for instance diffusion terms. In this paper, we present a complete set of rate equations, which describe all major characteristics of defect creation. The coupled rate equations are based on an exponential distribution of barrier states and barrier lowering due to the bandtail carriers. Due to their coupled nature, an analytical solution seems to be impossible. Therefore, they will be solved numerically and the contributions of different parts will be analysed individually to gain insight into their importance.

A more detailed description of our work will be published elsewhere \([9]\).

2. Experimental results

Bias stress experiments have been carried out on n-type, silicon-nitride gate insulator a-Si:H TFTs deposited at 300 °C on crystalline silicon wafer. The preparation conditions were reported elsewhere \([10]\). The TFTs have been annealed to 500 K before the stress experiment. A crucial aspect of the threshold voltage shift $\Delta V_g(t)$ is its super-linear behavior on the gate bias over initial threshold $V_g(t) - V_i$, i.e., the number of bandtail carriers $N_{BT}$ ($t$). This is manifested in Eq. (5) by the power $\alpha$ \([6]\). Experimentally, the power $\alpha$ can be determined by constant-current stress ($N_{BT} = \text{const}$) for which the kinetics have a power-law behavior for short and medium stressing times (Eq. (5)).

Fig. 1 shows $\Delta V_g(t)$ during constant-current stress for short stressing times as a function of the applied gate bias over initial threshold $V_g(t)$ \([11]\). Two different TFTs have been chosen, one with a very low mobility $\mu$ of 0.2 cm$^2$/V/s, another with a high mobility $\mu$ of 1.3 cm$^2$/V/s. For both TFTs, the threshold voltage shift $\Delta V_g(t)$ dependence on the gate bias over initial threshold $V_g(t) - V_i$ is super-linear, with the power $\alpha$ lying typically between 1.5 and 1.9.

![Fig. 1. Threshold voltage shift $\Delta V_g$ as a function of gate bias $V_g$ over initial threshold voltage $V_i$ for two samples (■: $\mu = 0.2$ cm$^2$/V/s, •: $\mu = 1.3$ cm$^2$/V/s). The constant-current stressing time was 1000 s at 80 °C.](Image)
3. Modelling

For the modelling, we apply an exponential barrier model for carrier-induced defect creation. The exact microscopic mechanism is not important since our model holds for different possible mechanisms: breaking of a silicon–silicon bond or emission of hydrogen out of an isolated silicon–hydrogen bond (Si–H) or a doubly hydrogenated silicon–silicon bond (SiHHSi or H₂). We therefore refer to the initial bond in the following as a precursor bond. The only two ingredients are an exponential distribution of barrier states \( N_A^*(E^*) = N_0 \exp[-(E_M - E^*)/kT_0] \) and a barrier lowering \( \Delta \) due to the bandtail carrier density \( n_{BT} : \Delta = E_{Form} + kT \ln(n_{BT}) \). Here, \( E_M \) corresponds to the energy to break a relaxed precursor bond and \( E_{Form} \) is the formation energy of a neutral defect. The rate of creating defects \( dN_D/dt \) for an energy barrier, \( E^* \), is

\[
\frac{dN_D(E^*, t)}{dt} = R_f(E^*, t)N_A(E^*, t) - R_b(E^*, t)N_D(E^*, t),
\]

where \( N_A \) is the number of precursor bonds, \( R_f \) and \( R_b \) the forward and backward reaction rate, respectively. \( N_A \) and \( N_D \) are related to each other by conservation of the total number of bonds \( N_A = N_D(t) + N_A(t) \). The bandtail carrier density triggers a defect creation event. Therefore the activation energy for the forward reaction rate is lowered by \( \Delta \). It is rather unlikely that two electrons will be localized on one precursor bond under typical electron densities \( 10^{19} \text{ cm}^{-3} \) and localization length of \( 10 \) \( \text{Å} \), so that the activation energy has only once the barrier lowering energy \( \Delta \). However, in the final state, one precursor bond will always create two defects, which under electron accumulation are both charged. Thus, the site \( B \) is lowered twice \( (2\Delta) \) (Fig. 2). Notice that one defect creation site, \( B \), corresponds to two electronically active states. Thus, we obtain for the forward and backward reaction rates \( R_f \) and \( R_b \)

\[
R_f(t) = v_f n_{BT} \exp \left( -\frac{E^* - E_{Form}}{kT} \right)
\]

\[
= v_f n_{BT} \exp \left( -\frac{E^* - E_{Form}}{kT} \right)
\]

(5)

and

\[
R_b(t) = v_b \exp \left( -\frac{E^* - 2E_{Form} + \Delta}{kT} \right)
\]

\[
= v_b n_{BT}^{-1} \exp \left( -\frac{E^* - E_{Form}}{kT} \right)
\]

(6)

Inserting Eqs. (5) and (6) in Eq. (4), and considering that the total number of sites \( N_A^* \) is constant, one obtains for the rate of created defect per energy barrier \( E^* \).

\[
\frac{dN_D(E^*, t)}{dt} \exp \left( -\frac{E^* - E_{Form}}{kT} \right)
\]

\[
\times \left\{ n_{BT}N_0 \exp \left( \frac{E^* - E_{Form}}{kT_0} \right) - N_D(E^*, t) \left[ n_{BT} + \frac{v_b}{v_f} n_{BT} \right] \right\}.
\]

We have performed numerical calculations for an array of 30 energy levels, \( E^* \), for a constant-voltage stress situation, i.e., \( n_{BT}(t) = N_0 = 2 \sum_{i=1}^{30} N_D(E^*_i, t) \). In [12], we have shown that this numerical fit has a very good agreement to the stretched hyperbola shape of threshold voltage shifts. Here, we analyse if the model correctly reproduces the super-linear bandtail carrier dependence. Therefore, we have determined in the short time stressing limit the threshold voltage shift for different initial bandtail carrier densities. We have
numerically verified that after about 1000 s, the bandtail carrier density remains essentially unchanged.

Varying the initial bandtail carrier density over one order of magnitude, we derive by a linear fit in a double logarithmic plot the coefficient \( a \) which turns out to be about 1.5 in good agreement with the experiment (Fig. 3). The parameters used in the calculation are \( \beta = 0.53 \), \( E_M = 1.045 \text{ eV} \), attempt-to-escape frequencies \( v_f = v_b = 10^{10} \text{ Hz} \). The formation energy \( E_{\text{Form}} \) has been set to zero since it would only change the absolute number of created defects, not the time or bandtail carrier dependence of the kinetics (Eq. (7)).

4. Discussion

There are at least two key experimental characteristics of defect creation, which every model has to describe: the stretched hyperbola time behaviour [4–8] and the super-linear bandtail carrier dependence of the defect creation rate [6,7]. To understand the origin of \( \alpha \approx 1.5 \), we have analysed in more detail the impact of the key contributions on our rate equations. These are the forward reaction rate, the backward reaction rate and the charge states manifested by the barrier lowering \( \Delta \) and the amount of defects created per precursor bond.

If we consider the forward reaction rate only, the carrier-induced barrier lowering \( \Delta \) leads to an activation energy lowering of the forward reaction rate. (Fig. 2). Even though, we do not change the formation energy of defect creation, there is a net increase in the defect density due to the exponential density of states. The defect creation rate is proportional to \( n_{\text{BT}}^a \) due to the Boltzmann approximation in an exponentially increasing density of states: the barrier lowering is \( \Delta/kT_0 \) and \( \Delta \) is proportional to \( kT \ln(n_{\text{BT}}) \). Thus, the impact of \( n_{\text{BT}} \) on the defect creation rate is modified by the power \( \alpha \approx \beta = T/T_0 \). This would lead to values of \( \alpha \approx 0.5 \) in disagreement with the experimental data (Figs. 1 and 3).

If we consider both the forward and backward reaction, the barrier state \( A \) is lowered by \( \Delta \) and the final state \( B \) is lowered by \( \Delta \) (Fig. 2). Thus, the forward reaction rate is increased whereas the backward reaction is decreased. There is now in addition to prior case, an increase of the formation energy of defects by \( \Delta \). This leads to an increased efficiency of the bandtail carrier density on the defect creation rate since \( \Delta \) depends on the bandtail carrier density and an approximate relationship of \( \alpha \approx 2\beta \) is obtained due to the exponential density of states. This is confirmed by numerical modelling in the short time limit, which yields values of \( \alpha \approx 1 \) (Fig. 3).

If we finally also consider that every defect site \( B \) consists of two electrically active defects, the forward reaction rate is lowered by \( \Delta \) whereas the backward reaction rate is lowered by \( 2\Delta \) (Fig. 2). Thus, the formation energy is increased by \( 2\Delta \). This implies that during the period of breaking the bond only one electron will be located on the weak precursor bond. This is a reasonable approximation since there is a low probability of a doubly occupied weak bond due to coulomb interaction and the ratio of accumulated electrons to weak bond (typically about \( 10^{-2} \)). The net effect is an increased quenching of the backward reaction rate by the bandtail carriers density. This doubles the bandtail carrier efficiency of the backward reaction.

Fig. 3. Numerical simulation of the threshold voltage shift as a function of the gate bias for three different models: (■) taking into account only the forward reaction only; (●) taking into account the forward and backward reaction only; (▼) taking into account the forward and backward reaction and the charge states (Eq. (7), Fig. 2). The bandtail carrier dependence of the defect creation rate goes with the power of \( \alpha \) shown next to the curves. Parameters: \( kT = 30.4 \text{ meV}, kT_0 = 62 \text{ meV}, t = 1000 \text{ s} \).
on the defect creation rate leading to a super-linear value, given by $x \approx 3\beta$, in line with our numerical modeling (Fig. 3).

The relationship $x \approx 3\beta$ is seen to hold, for different TFTs, with different values of $\beta$. For example, for a high mobility TFT, with an Urbach energy $kT_0$ of typically 50 meV [10], we obtain for $kT = 30$ meV, $\beta = 0.6$ and $x \approx 3\beta = 1.8$. For a low mobility TFT, with typically $kT_0 = 60$ meV, $\beta = 0.5$ and $x \approx 3\beta = 1.5$. This is in excellent agreement with our experimental data (Fig. 1).

5. Conclusion

A set of coupled rate equations has been developed to describe the defect creation kinetics in thin film transistors. These rate equations are only based on an exponential distribution of barrier states and a carrier-induced barrier lowering. Solving these equations, numerically, all important characteristics can be modelled, namely, the stretched hyperbola shape and the super-linear bandtail carrier dependence. We have shown that the latter characteristic shows a very good agreement between theory and experiment. In particular, the bandtail carrier dependence of the defect creation rate goes with the power $x$, where $x \approx 3\beta$.

References