Physics of Complex Systems, 2025, vol. 6, no. 1
www.physcomsys.ru

Physics of Semiconductors. Semiconductors

UDC 621.382.323

EDN TUEBOO
https://www.doi.org/10.33910/2687-153X-2025-6-1-26-34

Modelling the behavior of metal-oxide-semiconductor structures under thermal field treatment

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For citation: Aleksandrov, O. V., Morozov, N. N. (2025) Modelling the behavior of metal-oxide-semiconductor structures under thermal field treatment. *Physics of Complex Systems*, 6 (1), 26–34. https://www.doi.org/10.33910/2687-153X-2025-6-1-26-34 EDN TUEBOO

Received 26 August 2024; reviewed 9 October 2024; accepted 9 October 2024.

Funding: The study did not receive any external funding.

Abstract. A quantitative model of the behavior of metal-oxide-semiconductor (MOS) structures subjected to thermal field treatment, particularly in the accumulation and recovery modes of mobile charge in the gate dielectric, is presented. The mobile charge transport is modelled based on ion trapping on polyenergetic defects with a spectrum of binding energies. The time-dependent shifts in the threshold voltage of the MOS structures under positive and subsequent negative gate biases are simulated. The proposed model accounts for both symmetric and asymmetric behaviours observed in MOS structures containing Na^+ ions. Additionally, the model determines the range of binding energies, trap concentrations, and the spatial localization of traps.

Keywords: MOS structure, gate dielectric, mobile charge, thermal field treatment, dispersion transport, polyenergetic traps, amorphous silicon dioxide, modeling

Introduction

Positive Bias Temperature Instability (PBTI) may be observed during thermal field treatment (TFT) of MOS structures with a positive gate voltage (Grasser 2014; Zhang et al. 2022). This phenomenon is associated with the transport of mobile impurity ions of alkaline earth metals, primarily sodium (Na^+), from the gate to the silicon (Si) substrate in the electric field of the gate dielectric. Two primary models have been proposed to describe the kinetics of mobile charge accumulation during TFT: Snow's diffusion model (Snow et al. 1965), and Hofstein's interface trapping model (Hofstein 1966). In Show's model, the transfer of mobile charge from the gate to the Si substrate is governed by the diffusion and drift rates of free impurity ions in the dielectric. The accumulated mobile charge is proportional to the square root of the TFT duration:

$$Q \sim \sqrt{t}. \tag{1}$$

In Hofstein's model, the rate of charge accumulation is determined by the release rate of impurity from the interphase boundary (IPB) between the dielectric and the gate. In this case:

$$Q = Q_0(1 - \exp(-t/\tau)), \tag{2}$$

where Q_0 is the initial charge, τ is the time constant, $\tau^{-1} = \nu \exp(-\frac{E}{kT})$, ν is the frequency factor, E is the binding energy, T is the TFT temperature, k is the Boltzmann constant ($k = 8.617 \times 10^{-5}$ eV/K).

When the polarity is reversed, the charge near the Si substrate decreases (or is restored) as the mobile ions return to the gate. According to the diffusion model, this process should occur at the same rate as the accumulation, resulting in symmetric behavior. Conversely, the boundary capture model suggests that restoration occurs much faster than accumulation, reflecting asymmetric behavior due to the high speed of free impurity transport. In practice, both behaviors are observed, and the kinetics of accumulation and restoration deviate from the simple dependencies described by equations (1) and (2) (Hofstein 1966; Snow et al. 1965).

These deviations may be attributed to the capture of impurity by traps in the dielectric, which slows the rate of impurity ion transfer (Aleksandrov, Morozov 2023). Moreover, in the case of amorphous silicon dioxide, these traps are not monoenergetic, but polyenergetic, exhibiting a distribution (or dispersion) in binding energies. The dispersive transport of charge carriers in amorphous materials can be modeled by multiple capture events involving polyenergetic traps (Noolandi 1977). For amorphous silicon dioxide, these traps may include oxygen vacancies or other structural defects.

The aim of this work is to develop a quantitative model for the behavior of MOS structures during TFT, focusing on the capture of mobile impurity ions by polyenergetic traps in the gate oxide. The model also simulates time-dependent shifts in the threshold voltage.

Model equations

The gate dielectric of the MOS structure (amorphous silicon dioxide, SiO_2) contains structural defects, such as oxygen vacancies, which can serve as polyenergetic traps for mobile impurity ions. It is assumed that during their transport, impurity ions can be captured by neutral traps, T_i^0, within the volume of silicon dioxide, leading to the formation of positively charged complexes NT_i^+:

$$N^+ + T_i^0 \underset{k_{2i}}{\overset{k_{1i}}{\rightleftarrows}} NT_i^+, i = 1,2\ldots n, \tag{3}$$

where k_{1i} and k_{2i} are the rate constants for the direct and reverse reactions of the impurity with the i-th trap. The system of diffusion-drift continuity equations and the Poisson equation, describing the transport of impurity ions and their capture by polyenergetic traps in accordance with reaction (3), is as follows:

$$\frac{\partial C_N^+}{\partial t} = D\frac{\partial^2 C_N^+}{\partial x^2} - \mu\frac{\partial}{\partial x}(C_N^+ \cdot E) - C_N^+ \sum_{i=1}^{n} k_{1i} C_{Ti}^0 + \sum_{i=1}^{n} k_{2i} C_{NTi}^+, \tag{4}$$

$$\frac{\partial C_{NTi}^+}{\partial t} = -\frac{\partial C_{Ti}^0}{\partial t} = k_{1i} C_{Ti}^0 C_N^+ + k_{2i} C_{NTi}^+, i = 1,2\ldots n, \tag{5}$$

$$\frac{\partial^2 V}{\partial x^2} = -\frac{\rho}{\varepsilon\varepsilon_0} = -\frac{q}{\varepsilon\varepsilon_0}(C_N^+ + \sum_{i=1}^{n} C_{NTi}^+), \tag{6}$$

where x is the coordinate ($x = 0$ on the Si-SiO_2 IPB and $x = d$ on the SiO_2-metal gate IPB, d is the oxide thickness); t is the TFT time; C_N^+ is the concentration of free impurity ions N^+, C_{Ti}^0 is the concentration of neutral traps T_i^0, C_{NTi}^+ is the concentration of positively charged complexes NT_i^+; V is the potential distribution in the dielectric; E is the electric field strength, $E = -dV/dx$; D is the diffusion coefficient of free ions; μ is the ion mobility; ($\mu = D/(kT)$ according to the Einstein relation), q is the elementary charge ($q = 1.6 \cdot 10^{-19}$ C); ε is the relative permittivity of the dielectric ($\varepsilon(SiO_2) = 3.9$); ε_0 is the electric constant ($\varepsilon_0 = 8.85 \cdot 10^{-12}$ F/m).

The mobility of impurity ions in amorphous SiO_2 is described by the Arrhenius equation:

$$\mu = \mu_0 \exp(-\frac{E_a}{kT}), \tag{7}$$

where μ_0 is the pre-exponential factor, and E_a is the activation energy. The mobility of Na^+ ions in SiO_2 was determined in (Stagg 1977) using the thermally stimulated ion current method in the fields up to $E = 5 \times 10^5$ V/cm, $\mu_0 = 1.05$ cm²/V×s, $E_a = 0.66$ eV.

We assume that the capture of an ion by different traps T^0_i is equally probable, and under diffusion limitation, the rate constant of the forward reaction (3) is determined by the diffusion coefficient of free ions: $k_{1i} = k_1 = 4\pi RD$, where R is the effective radius of ion capture by a trap (we assume $R \cong 1$ Å). The reverse reaction occurs at a rate that depends on the binding energy of the ion with the i-th trap E_{bi}: $k_{2i} = \nu \exp(-\frac{E_{bi}}{kT})$, where ν is the vibration frequency of atoms, $\nu = 10^{12}$ s^{-1}. The binding energy is distributed within the range from E_{b1} to E_{bn}: $E_{bi} = E_{b1} + \Delta E_{bi} \cdot (i-1), i = 1,2\ldots n,$ where $\Delta E_{bi} = dE_{bi} = \frac{E_{bn} - E_{b1}}{n}$, is the energy increment.

We assume that the distribution of traps by energy follows an exponential form, characteristic of amorphous materials (Arkhipov, Rudenko 1982):

$$\frac{\partial C_{Ti}(x, E_{bi})}{\partial E_{bi}} = C_T(x)\frac{1}{E_0}\exp(-\frac{E_{bi}}{E_0}), i = 1,2\ldots n, \tag{8}$$

where E_0 is the characteristic energy corresponding to the width of the energy distribution of traps, $C_{Ti}(x, E_{bi})\varnothing E_{bi}$ is the concentration of traps with energies from E_{bi} to $E_{bi} + \Delta E_{bi}$, and $C_T(x)$ is the distribution of traps along the coordinate without taking into account the energy distribution, which we assume to be exponential near both IPBs:

$$C_T(x) = \frac{Q'_{TSi}}{L_{Si}}\exp(-\frac{x}{L_{Si}}) + \frac{Q'_{TMe}}{L_{Me}}\exp(-\frac{d-x}{L_{Me}}), \tag{9}$$

where Q'_{TSi}, Q'_{TMe} are the integral concentrations of traps near the Si-SiO_2 and SiO_2-gate IPBs, respectively, without taking into account the energy distribution, and L_{Si} and L_{Me} are the widths of the corresponding exponential distributions of traps.

By summing equations (8) over energies and replacing the sum with an integral, we obtain an expression for the total concentration of traps in the selected range E_{b1} — E_{bn}:

$$\begin{aligned} C_{Tsum}(x) &= \sum_{i=1}^{n} C_{Ti}(x, E_{bi})\Delta E_{bi} = \int_{E_{b1}}^{E_{bn}} C_{Ti}(x, E_{bi})dE_{bi} = \\ &= C_T(x)(\exp(-\frac{E_{b1}}{E_0}) - \exp(-\frac{E_{bn}}{E_0})). \end{aligned} \tag{10}$$

The integral concentrations of traps in this range from equations (9) and (10) can be expressed as:

$$Q_{TSi} = Q'_{TSi}(\exp(-\frac{E_{b1}}{E_0}) - \exp(-\frac{E_{bn}}{E_0})), \tag{11}$$

$$Q_{TMe} = Q'_{TMe}(\exp(-\frac{E_{b1}}{E_0}) - \exp(-\frac{E_{bn}}{E_0})). \tag{12}$$

We assume that at the initial moment of time, the charged complexes are in equilibrium with free impurity ions and neutral traps:

$$k_1 C^0_{Ti} C^+_N = k_{2i} C^+_{NTi}, i = 1,2\ldots n, \tag{13}$$

Replacing $C_{Ti}^{0}(x) = C_{Ti}^{0}(x, E_{bi})\Delta E_{bi} - C_{NTi}^{+}(x)$, $\sum_{i=1}^{n} C_{NTi}^{+}(x) = C_{Nsum}^{+}(x) - C_{N}^{+}(x)$ and summing (14) over i, we get:

$$C_{N}^{+}(x)\left(1 + \sum_{i=1}^{n} \frac{C_{Ti}(x, E_{bi})\Delta E_{bi}}{C_{N}^{+}(x) + \dfrac{k_{2i}}{k_1}}\right) = C_{Nsum}^{+}(x). \tag{14}$$

Solving equation (14) using the bisection method, we find the distributions of $C_{N}^{+}(x)$, $C_{Ti}^{0}(x)$, and $C_{NTi}^{+}(x)$ in the equilibrium for a given TFT temperature at the initial time $t = 0$.

The boundary conditions are assumed to be a constant gate bias and dielectric boundaries that reflect the impurity ions:

$$V(d,t) = V_G, \tag{15}$$

$$j(0,t) = j(d,t) = 0, \tag{16}$$

where j is the flux of impurity ions, $j(x,t) = -D\dfrac{\partial C_{N}^{+}}{\partial x} + \mu C_{N}^{+} E$.

To assess the influence of mobile ions accumulation on the behavior of the MOS structure, the effective amount of impurity ΔQ_{ot} and the threshold voltage shift ΔV_{th} (equal to the flat-band voltage shift ΔV_{fb}) near the SiO_2-Si MOS IPB are calculated:

$$\Delta Q_{ot}(t) = \int_{0}^{d} \left(C_{Nsum}^{+}(x,t) - C_{Nsum}^{+}(x,0)\right)\frac{d-x}{d}\,dx, \tag{17}$$

$$\Delta V_{th}(t) = \frac{q}{C_{ox}}\Delta Q_{ot}(t), \tag{18}$$

where $C_{ox} = \varepsilon\varepsilon_0/d$ is the specific capacitance of the dielectric.

The system of equations of model (4)–(6) with the initial condition (14) and boundary conditions (15)–(16), taking into account equation (8), was solved numerically using both explicit and implicit difference schemes.

Calculation results and discussion

The calculation results were compared with the experimental data from (Kriegler, Devenyi 1973) and (Snow et al. 1965) on the TFT of MOS structures contaminated with Na^+ ions. In (Kriegler, Devenyi 1973), the MOS structure had an aluminum gate, with the gate oxide formed by thermal oxidation in dry oxygen at a temperature of 1150 °C, resulting in a thickness of 120 nm. Sodium was introduced into the structure during the deposition of aluminum at an approximate concentration of 10^{12} cm^{-2}. TFT measurements were performed at temperatures of 75 °C, 120 °C, and 175 °C, with a gate bias of $V_G = +2$ V in the charge accumulation mode and at $V_G = -1$ V in the subsequent recovery mode.

Figure 1 shows the kinetics of threshold voltage shift as a function of time in the accumulation mode on the silicon substrate. Curves 1–3 represent experimental dependences from (Kriegler, Devenyi 1973), while curves 1’–3’ show calculations for monoenergetic traps at $E_b = 1.14$ eV following (Aleksandrov, Morozov 2023), and curves 1”–3” represent calculations for polyenergetic traps at $E_{b1} = 0.9$ eV, $E_{bn} = 1.4$ eV, $E_0 = 0.25$ eV. The comparison in Figure 1 reveals that calculations incorporating polyenergetic traps, in contrast to those based on monoenergetic traps, better represent the experimental data.

The lower limit of the energy range of the traps was initially set to the activation energy of Na^+ ions mobility ($E_{b1} = E_a = 0.66$ eV, as reported by (Stagg 1977)), but was subsequently adjusted to 0.9 eV, since at lower values of E_{b1} the calculation results do not change, due to the rapid depletion of traps with small E_{b1}. The upper limit of the range $E_{bn} = 1.4$ eV was taken to be equal to the highest activation energy experimentally recorded for the diffusion of sodium ions following (Sugano et al. 1968). The number of trap energy levels within the range was taken to be $n \geq 30$, ensuring that the solution became independent of n.

The obtained range of 0.9-1.4 eV corresponds to the activation energy range for the 'slow' diffusion of sodium ions, as described in (Verwey et al. 1990). The narrow distribution of traps near the gate ($L_{Me} = 2$ nm) was selected to reflect the fact that, at negative V_G, no significant shift in the threshold voltage was observed during TFT, with the voltage shift measured as $\Delta V_{th} = 3$ mV at $T = 120$ °C, $V_G = -2$ V). The appearance of the calculated dependences at temperatures of 75 °C and 120 °C resembles the root function (1) of Snow's model (Snow et al. 1965), while at 175 °C, the behavior aligns more closely with the function (2) of Hofstein's model (Hofstein 1966).

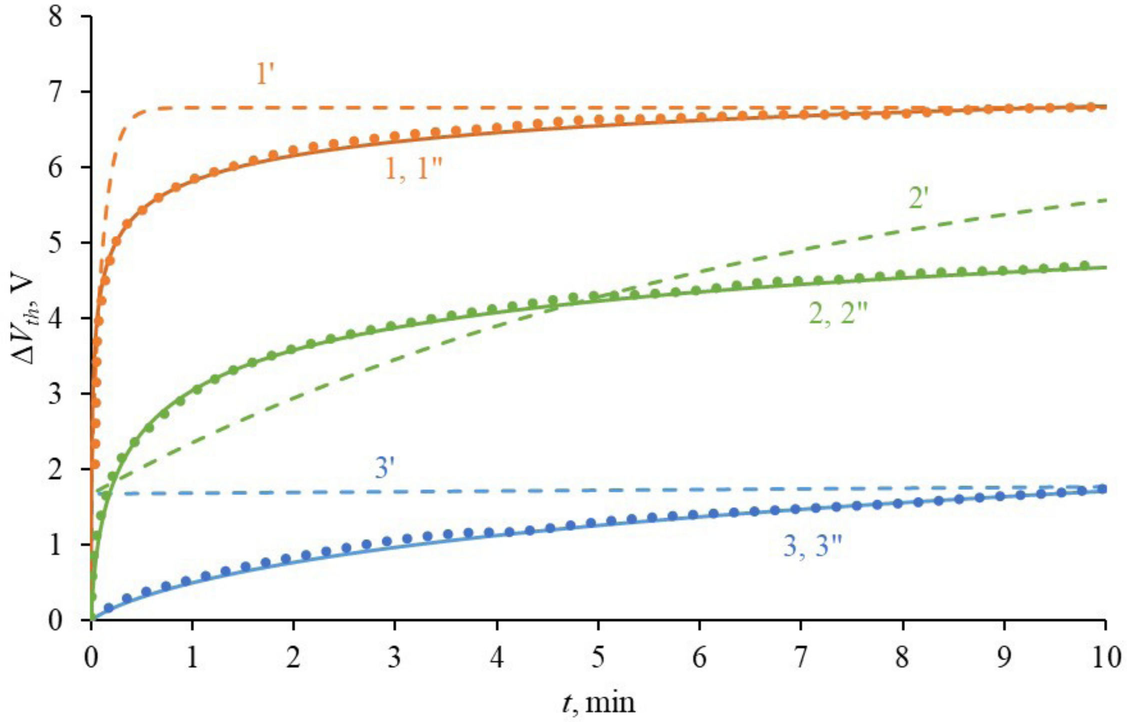

Fig. 1. Dependences of $\Delta V_{th}(t)$ during TFT (accumulation mode $V_G = +2$ V, $d = 120$ nm) at temperatures, °C: 1, 1', 1" — 175; 2, 2', 2" — 120; 3, 3', 3" — 75 °C. Curves 1–3 — experimental data from (Kriegler, Devenyi 1973); 1'–3' — calculations for monoenergetic traps ($E_b = 1.14$ eV, $Q^{+}_{N\,Me} = 1.25 \times 10^{12}$ cm^{-2}, $Q_{TMe} = 9.4 \times 10^{11}$ cm^{-2}); 1"–3" — calculations for polyenergetic traps ($E_{b1} = 0.9$ eV, $E_{bn} = 1.4$ eV, $E_0 = 0.25$ eV, $Q^{+}_{N\,Me} = 1.4 \times 10^{12}$ cm^{-2}, $Q_{TMe} = 2.13 \times 10^{12}$ cm^{-2})

In (Snow et al. 1965), the MOS structure was contaminated with sodium prior to sintering the aluminum gate. The gate oxide thickness was 200 nm. TFT measurements were performed at temperatures of 80 °C, 100 °C, 120 °C, 140 °C, and 160 °C with a gate bias of $V_G = +10$ V for one hour.

Figure 2 shows the experimental data (symbols 1–4) from (Snow et al. 1965) and the calculated dependences (curves 1'–4') between the effective charge and the $Q_{ot}(t^{1/2})$ during TFT. It is evident from Figure 2 that the experimental dependences from (Snow et al. 1965) deviate from both Snow's model (1) and Hofstein's model (2), but are satisfactorily described by the proposed model based on polyenergetic traps, with the same parameters used in Figure 1 as in (Kriegler, Devenyi 1973), i. e., $E_{b1} = 0.9$ eV, $E_{bn} = 1.4$ eV, $E_0 = 0.25$ eV.

The kinetics of the threshold voltage change during the recovery mode at $V_G = -1$ V (following the accumulation mode at $V_G = +2$ V, $T = 120$ °C, $t = 10$ min) is shown in Figure 3 (curve 1) based on the data from (Kriegler, Devenyi 1973). Curves 2 and 3 show the calculation using the polyenergetic trap model with the same trap parameters at the gate as those in Figure 1. These calculations are performed both in the absence of traps in silicon (curve 2, $Q_{TSi} = 0$) and with a small number of traps present (curve 3, $Q_{TSi} = 2.36 \times 10^{11}$ cm^{-2}). The trap parameters in silicon are identical to those at the gate ($E_{b1} = 0.9$ eV, $E_{bn} = 1.4$ eV, $E_0 = 0.25$ eV), except for the distribution width, which was taken to be $L_{Si} = 5$ nm, according to the data from (DiMaria 1977).

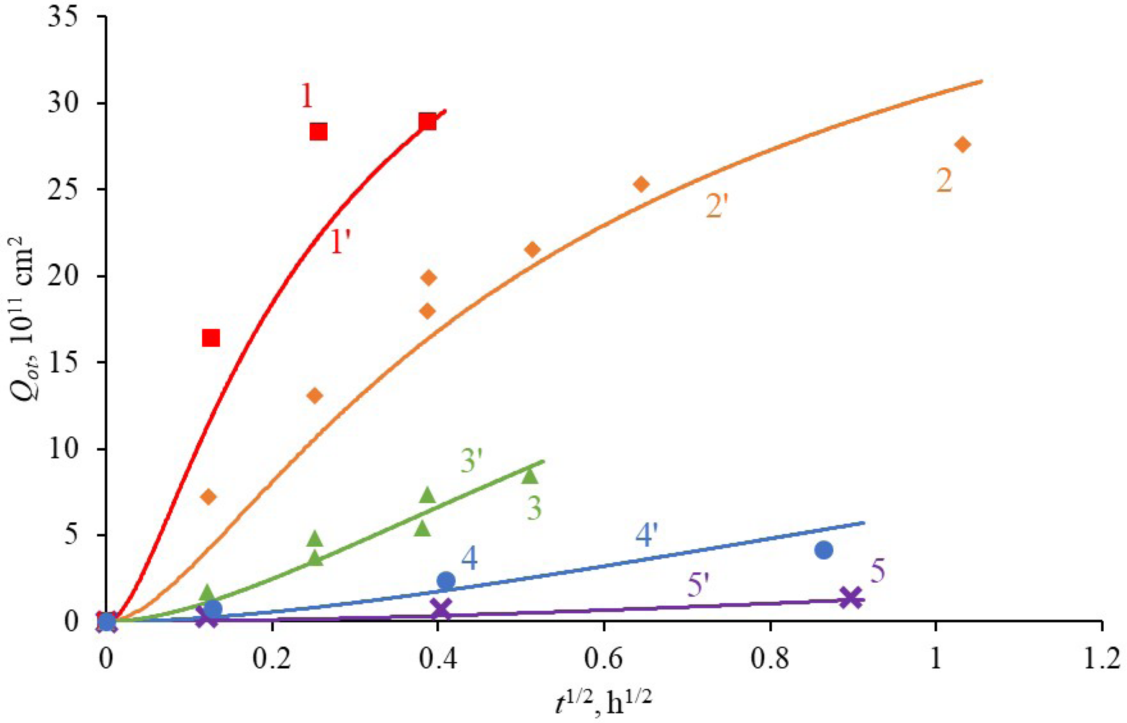

Fig. 2. $Q_{ot}(t^{1/2})$ dependences during TFT (accumulation mode V_G = +10 V, d = 200 nm) for temperatures, °C: 1, 1’ — 160; 2, 2’ — 140; 3, 3’ — 120; 4, 4’ — 100; 5, 5’ — 80. Curves 1–5 — experimental data (Snow et al. 1965); 1’–5’ — calculation for polyenergetic traps (E_{b1} = 0.9 eV, E_{bn} = 1.4 eV, E_0 = 0.25 eV, Q_{N^+Me} = 5.3 × 10^{12} cm^{-2}, Q_{TMe} = 2.24 × 10^{13} cm^{-2})

As shown in Figure 3, recovery occurs much faster than accumulation, indicating asymmetric behavior. The initial rapid voltage drop is caused by the drift of free impurity from the Si-SiO$_2$ IPB, with the slope of this drop characterized by the mobility of free ions. In the case of no traps near silicon (curve 2), at $t > 0.2$ s, the threshold voltage is completely restored to $V_{th} = 0$ ($|\Delta V_{th}| = \Delta V_{th}$ (at $+V_G$)). However, when traps are present near silicon (curve 3), the threshold voltage does not fully recover, as the impurity ions are captured by traps near the boundary with silicon. Among the available literature data on the diffusion coefficient of free sodium ions (Greeuw, Verwey 1984; Hofstein 1967; Kriegler, Devenyi 1976; Stagg 1977; Sugano et al. 1968; Verwey et al. 1990), the data from (Stagg 1977) provide the best correlation with the experimental observations in the region of fast drift.

The asymmetry observed in the charge accumulation and recovery dependencies $\Delta V_{th}(t)$ in Figures 1–3 within the framework of the model can be explained by two factors: first, the initial position of Na$^+$ ions on traps near the gate, and, second, the relatively low concentration of traps near the Si-SiO$_2$ IPB (Q_{TSi} = 2.36 × 10^{11} cm^{-2}) for silicon oxide obtained by thermal oxidation in dry oxygen.

In contrast, when ‘chlorine’ oxides are used, which are obtained by thermal oxidation in the presence of HCl vapor, a more symmetrical accumulation-reduction time dependences are observed during TFT. This symmetry is attributed to an increase in the concentration of traps near silicon, which slows down the drift of sodium ions during the reduction mode under a negative bias. In (Kriegler, Devenyi 1973), along with standard samples with oxide produced by thermal oxidation in dry oxygen (see Figs. 1 and 3), samples with chlorine oxide were also studied. The thermal oxidation of these samples was performed at a temperature of 1150 °C in an atmosphere containing 6% HCl: O$_2$. The oxide films formed were 115 nm thick. TFT in the recovery mode was carried out at temperatures of 250 °C, 225 °C, 200 °C, and 175 °C with a gate bias of V_G = –2 V (after applying V_G = +2 V at T = 200 °C for t = 5 min). The amount of charge $Q_{ion} = qQ_{ot}A$ that moved from silicon with a negative bias to the gate with an area of A = 0.025 cm^2 was measured. Under a positive bias during the accumulation mode, the experimental dependences $\Delta V_{th}(t)$ for both the standard and chlorine oxides, as reported in (Kriegler, Devenyi 1973), were identical. This indicates that the defects induced by chlorine are concentrated near the SiO$_2$-Si IPB and do not impact the drift of sodium ions from the gate to silicon.

Figure 4 shows the calculated $Q_{ion}(t)$ dependencies for chlorine oxide in the reduction mode.

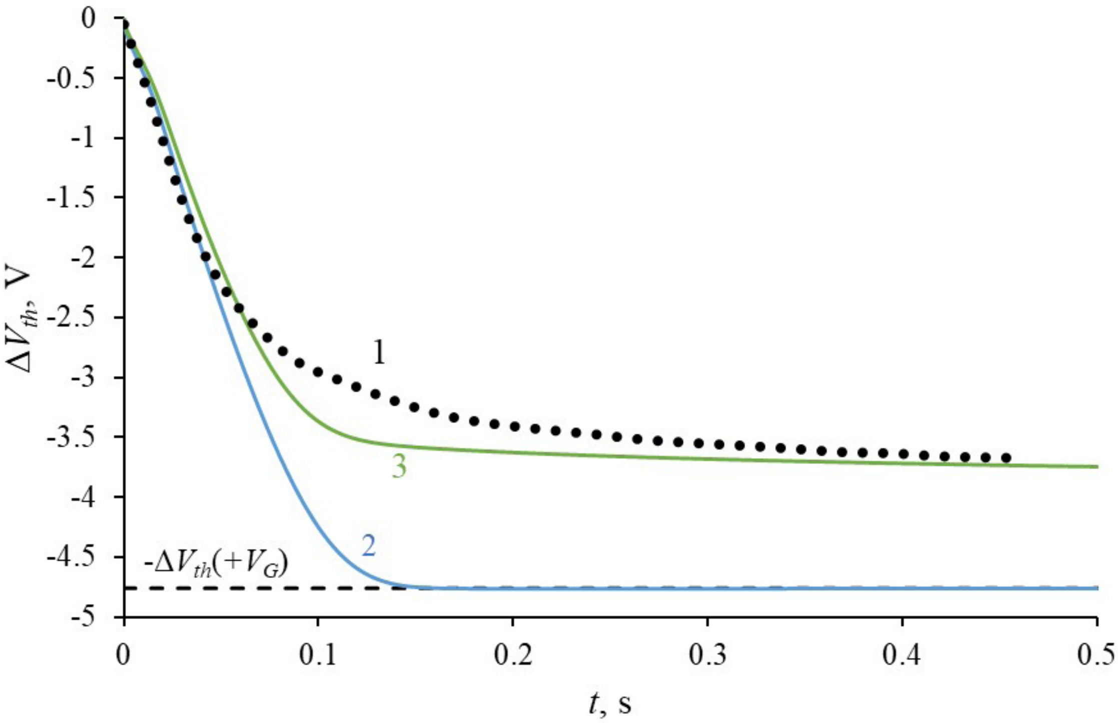

Fig. 3. Dependence of $\Delta V_{th}(t)$ during TFT (recovery mode, $V_G = -1$ V, $T = 120$ °C, $d = 120$ nm). Curve 1 — experimental data (Kriegler, Devenyi 1973); curve 2 — calculation based on the model with no traps near silicon, $Q_{TSi} = 0$; curve 3 — calculation based on the model with traps near silicon, $Q_{TSi} = 2.36 \cdot 10^{11}$ cm^{-2}, $L_{Si} = 5$ nm. The trap parameters near the gate are the same as those in Figure 1

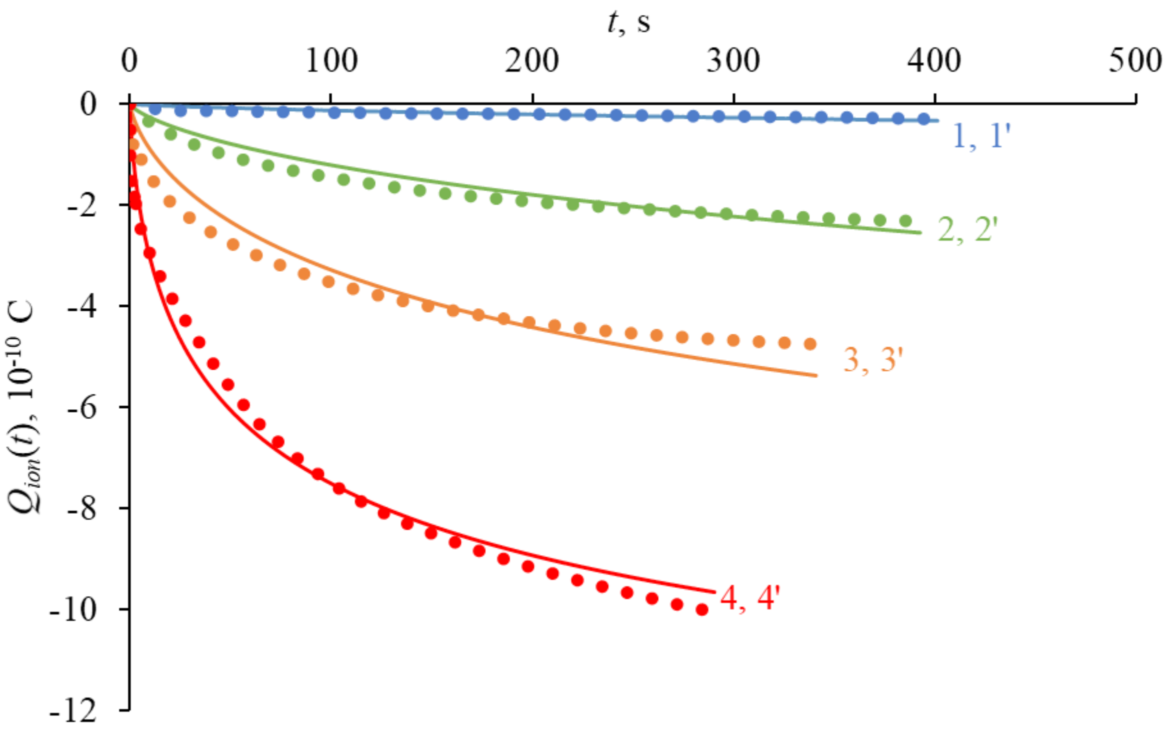

Fig. 4. $Q_{ion}(t)$ dependences during TFT (reduction mode, $V_G = -2$ V, $d = 115$ nm, $A \approx 0.025$ cm^2) for temperatures, °C: 1, 1' — 175; 2, 2' — 200; 3, 3' — 225; 4, 4' — 250. Curves 1–4 — experimental data (Kriegler, Devenyi 1973); 1'–4' — calculation for $Q_{N^{+}Si}$, cm^{-2}: 1' — 3.7×10^{11}; 2' — 4.6×10^{11}; 3' — 4.7×10^{11} cm^{-2}; 4' — 5.1×10^{11} ($Q_{TSi} = 3.51 \times 10^{12}$ cm^{-2}, $E_{b1} = 0.9$ eV, $E_{bn} = 2$ eV, $E_0 = 0.25$ eV, $L_{Si} = 5$ nm)

The calculation shows that, for the given parameters of the preliminary positive bias, almost all the impurity migrates from the gate to the substrate (Q_{Nsum} = 1.4 × 10^{12} cm^{-2}). Consequently, the recovery calculation was performed assuming an initial impurity distribution on traps near silicon in the local equilibrium state at the corresponding TFT temperatures. The experimental curves were obtained by varying $Q_N{}^+{}_{Si}$, while maintaining a constant number of traps near silicon Q_{TSi} = 3.5 × 10^{12} cm^{-2} (curve 1'–4'), using the same parameters of polyenergetic traps (E_0 = 0.25 eV, E_{b1} = 0.9 eV), but with a higher E_{bn} = 2 eV. The distribution width L_{Si} = 5 nm was taken from the experiment (DiMaria 1977). From the values obtained for curves 1'–4' ($Q_N{}^+{}_{Si}$ = (5.1 – 3.7) × 10^{11} cm^{-2}), it is evident that the integral amount of impurity Na$^+$ ions in the chloride oxide, when moving from silicon (with a negative bias), is less than when migrating to silicon (with a positive bias). This suggests neutralization of some Na$^+$ ions located on traps close to the SiO$_2$-Si IPB. As established in (Aleksandrov 2015; Dmitriev, Markin 1998), neutralization occurs due to the capture of electrons from the silicon substrate:

$$Na^+ + T^0 + e^- \underset{k_2'}{\overset{k_1'}{\rightleftarrows}} NT^0.$$

We assume that the formation of the inactive part of the impurity $Q_N' = Q_{Nsum} - Q_N$ is limited by the slower reaction of the impurity ions with the traps and is in equilibrium with them:

$$C_{NT}^0 = \frac{k_1'}{k_2'} C_N^+ C_T^0,$$

$$Q_N' = \frac{k_1'}{k_2'} Q_N Q_T / L,$$

$$k_2' = \frac{k_1'}{Q_N'} Q_N Q_T / L.$$

At $k_1' = k_1$, using the temperature dependence $k_2' = \nu' \exp(-\frac{E_b'}{kT})$, we find the binding energy of sodium in such neutral traps: E_b' = 0.82 eV, which is close to the lower limit of binding energies for polyenergetic traps (E_{b1} = 0.9 eV).

Conclusions

A quantitative model of the behavior of MOS structures during thermal field treatment has been developed based on the mechanism of capturing mobile impurity ions by polyenergetic traps in the bulk of the gate dielectric. At a positive gate voltage, the kinetics of charge accumulation in the IPB with silicon is determined by the rate of impurity ion release from polyenergetic traps in the IPB with a gate (Figs. 1 and 2). The parameters of these traps (E_{b1} = 0.9 eV, E_{bn} = 1.4 eV, E_0 = 0.25 eV), their concentrations, and the width of the localization region (L_{Me} = 2 nm) have been determined from experimental temperature dependences (Kriegler, Devenyi 1973; Snow et al. 1965).

Upon a subsequent change in polarity, the kinetics of charge recovery depends on the presence of traps near Si-SiO$_2$ IPB. In the absence of traps (Fig. 3, curve 2) or their low concentration for dry oxide (Fig. 3, curve 3), the recovery rate is high (showing asymmetric behavior) and is determined by the drift velocity of free impurity ions, as well as the internal field of ions. With a high concentration of traps in the chloride oxide near Si-SiO$_2$ IPB, the recovery rate becomes significantly slower (Fig. 4) and is comparable to the accumulation rate (indicating symmetric behavior). In this case, the recovery rate is determined by the rate of impurity ion release from polyenergetic traps near Si-SiO$_2$ IPB (Fig. 4). The parameters of the traps (E_{b1} = 0.9 eV, E_{bn} = 2.0 eV, E_0 = 0.25 eV), their concentrations, and the width of the localization region (L_{Si} = 5 nm) were determined by comparing the calculations with the experimental temperature dependences (Kriegler, Devenyi 1973). It was found that neutralization of a part of the ionized impurity occurs in chlorine oxide, and the binding energy of the Na impurity on such traps is calculated to be E_b' = 0.82 eV.

Conflict of Interest

The authors declare that there is no conflict of interest, either existing or potential.

Author Contributions

O. V. Alexandrov formulated the research problem, while N. N. Morozov carried out the calculations. Both authors analyzed the results and discussed the conclusions.

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