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Model of behavior of MOS structures during radiation-thermal treatments

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A quantitative model of the influence of radiation-thermal treatments on the resistance of MOS structures to ionizing radiation has been developed. The model is based on the interaction of holes formed during ionizing irradiation with hydrogen-containing and hydrogen-free traps in the gate dielectric. The capture of holes by hydrogen-containing traps stimulates the breaking of the hydrogen bond and their transformation into hydrogen-free traps with a smaller capture cross section. The model makes it possible to describe the increase in the radiation resistance of MOS structures during successive irradiation–annealing cycles while maintaining the integral concentration of traps.

Keywords: MOS structures, radiation-thermal treatments, ionizing radiation, radiation resistance.

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Introduction

Electron-hole pairs are generated in the dielectric of MOS structures in case of exposure to ionizing radiation (IR). Electrons with high mobility in silicon dioxide flow into the gate and into a semiconductor silicon substrate, and less mobile holes are trapped on hole traps, forming a positive volume charge in the dielectric (see monographs in Ref. [1,2] and reviews in Ref. [3–5]). Surface states are formed at the phase boundary (PB) Si–SiO_2 [3–5].

The radiation-thermal treatment (RTT) (IR + annealing) is one of the ways to increase the radiation resistance of silicon MOS integrated circuits [6–8]. The effect was associated with the relaxation of mechanical stresses under ionizing irradiation (IR) as a result of the breakage of valence bonds Si–O. The broken bonds are restored by a subsequent heat treatment to form a more stable atomic structure of silicon dioxide [6,8]. It is shown, however, that the effect of IR on MOS structures is not related to the direct interaction of radiation with the phase boundary Si–SiO_2 or the structural modification of SiO_2, but is associated with the generation of electron-hole pairs and hole transport [9]. It was assumed in Ref. [8] that the displacement of the drain-gate characteristics of MOS transistors observed in case of RTT was associated with a decrease of the density of trap centers in silicon oxide. However, a number of papers [10–12] showed that the change of the voltage shift of the flat zones of MOS structures or the threshold voltage of MOS transistors during annealing after IR is associated with the relaxation of the positive volume charge accumulated during IR with the preserved density of trap centers. Taking into account this circumstance, we believe that the increased radiation resistance of MOS structures in RTT may be the caused by the conversion of hydrogen-containing traps into hydrogen-free traps with a smaller capture cross section.

The purpose of this work is to develop a quantitative model of the behavior of MOS structures in case of RTT based on the mechanism of conversion of hydrogen-containing traps into anhydrous ones.

1. Experiment description

n- and *p*-channel MOS transistors produced using standard planar technology with a polysilicon gate were used for the study. The gate oxide with a thickness of 120 nm was grown in an atmosphere of dry oxygen with the addition of HCl vapors at a temperature of 1050°C for 80 min. The irradiation was carried out using GOT installation with a source of γ-radiation ^{137}Cs ($E_\gamma = 0.66$ MeV) at a radiation dose rate of 80 rad/s. The irradiation was carried out with a dose of $D = 10^6$ rad (SiO_2) with threshold voltage control at a dose of $5 \cdot 10^4$ rad. The drain-gate characteristics were recorded at each stage of irradiation–annealing and the threshold voltage shift was determined. The threshold voltage shift was divided into volumetric ΔV_{ot} and surface ΔV_{it} components by the mid-band gap method [13]. Annealing after IR was conducted at a temperature of 400°C for 30 min. The effect of the irradiation–annealing cycles on the drain-gate characteristics of *p*-MOS transistors is shown in Fig. 1.

The figure shows that the shift of the threshold voltage caused by the irradiation decreases with an increase of the number of cycles (curves *2, 4, 5*). Each annealing leads to the return of the drain-gate characteristics (curves *3, 6*) almost to the original level (curve *1*). That is, the volume charge and surface states introduced by irradiation are completely restored with the annealing used. It should be noted, as shown in Ref. [14], irradiation of MOS structures

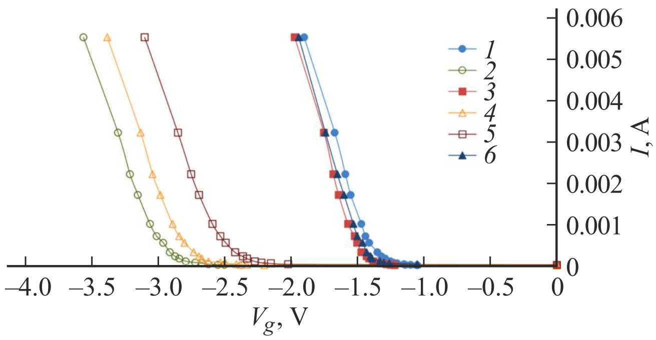

Figure 1. Effect of irradiation–annealing cycles on drain-gate characteristics of p-MOS transistors: *1* — initial characteristic; **2** — after the first irradiation ($D = 10^6$ rad); *3* — after the first annealing; *4* — after the third irradiation; *5* — after the sixth irradiation; *6* — after the sixth annealing.

with γ-quanta with energy of ~ 1 MeV is equivalent to low-energy (10 keV) X-ray irradiation, i.e. it is ionizing and does not result in the generation of displacement defects and Frenkel pairs in a gate dielectric SiO_2.

2. Model description

The exposure to ionizing radiation generates mobile charge carriers such as electrons and holes in the gate dielectric of the MOS structure, which interact with structural defects such as electron and hole traps. The main structural defects are oxygen vacancies $O_3 \equiv Si\bullet$ in amorphous thermal silicon dioxide SiO_2 (the sign $\equiv$ means saturated chemical bonds of silicon with three oxygen atoms, and the sign $\bullet$ means unsaturated broken silicon bond) [15]. Thermal silicon dioxide contains a high concentration of hydrogen (up to 10^{19}–$10^{20}\,cm^{-3}$ [16,17]). Hydrogen forms hydrogen-containing centers (TH) interacting with structural defects (T). It is shown in Ref. [18,19] that such hydrogen-containing defects $O_3 \equiv Si{-}H$ are the main hole traps in thermal silicon dioxide. The following reactions occur in the gate dielectric in case of IR. A positive volumetric charge is formed when holes are captured with anhydrous and hydrogen-containing traps:

$$T^0 + h^+ \xrightarrow{k1} T^+. \quad (1)$$

$$T\mathrm{H}^0 + h+ \xrightarrow{k2} T\mathrm{H}^+. \quad (2)$$

The capturing of the hole by hydrogen-containing traps stimulates the breakage of the hydrogen bond and their transformation into anhydrous traps with the release of a positive hydrogen ion:

$$T\mathrm{H}^0 + h^+ \xrightarrow{k3} T^0 + H^+. \quad (3)$$

Positively charged defects $T\mathrm{H}^+$ and T^+ become electronic traps:

$$T\mathrm{H}^+ + e^- \xrightarrow{k4} T\mathrm{H}^0, \quad (4)$$

$$T^+ + e^- \xrightarrow{k5} T_0. \quad (5)$$

The hydrogen ion produced by the reaction (3) can be captured back onto the trap T^0:

$$T^0 + \mathrm{H}^+ \xrightarrow{k6} T\mathrm{H}^+, \quad (6)$$

which slows down the migration of hydrogen ions in the dioxide.

The processes (1)–(6) are described by the following system of diffusion-kinetic equations and Poisson equations:

$$\frac{\partial p}{\partial t} = D_p \frac{\partial^2 p}{\partial x^2} - \mu_p \frac{\partial}{\partial x}(pE) - (k_2 - k_3)C^0_{TH}p - k_3 C^0_T p + G, \quad (7)$$

$$\frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} + \mu_n \frac{\partial}{\partial x}(nE) - (k_4 C^+_{TH} + k_5 C^+_T)n + G, \quad (8)$$

$$\frac{\partial C^+_H}{\partial t} = D^+_H \frac{\partial^2 C^+_H}{\partial x^2} - \mu^+_H \frac{\partial}{\partial_x}(C^+_H E) + k_2 C^0_{TH} p - k_6 C^0_T C^+_H, \quad (9)$$

$$\frac{\partial C^+_{TH}}{\partial t} = k_2 C^0_{TH} p - k_4 C^+_{TH} n + k_6 C^0_T C^+_H, \quad (10)$$

$$\frac{\partial C^0_{TH}}{\partial t} = -(k_2 + k_3)C^0_{TH} p + k_4 C^+_{TH} n, \quad (11)$$

$$\frac{\partial C^0_T}{\partial t} = k_3 C^0_{TH} p - k_1 C^0_T p - k_6 C^0_T C^+_H, \quad (12)$$

$$\frac{\partial C^+_T}{\partial t} = k_1 C^0_T p, \quad (13)$$

$$\frac{\partial^2 V}{\partial x^2} = -\frac{q}{\varepsilon\varepsilon_0}(C^+_{TH} + C^+_T + C^+_H + p - n), \quad (14)$$

where x — coordinate measured from the boundary of the dioxide with silicon ($0 \le x \le d$, d — dielectric thickness); t — irradiation time; n and p — concentrations of electrons and holes, respectively; D and μ with corresponding indices — diffusion coefficients and mobility of mobile components ($\mu_n = 20\,cm^2/(V{\cdot}s)$, $\mu_p = 4 \cdot 10^{-6}\,cm^2/(V{\cdot}s)$, $D^+_H = 1.0 \cdot \exp(-0.73/kT)\,cm^2/s$ [20], k — Boltzmann constant, T — absolute temperature), V — potential, E — electric field strength, $E = -dV/dx$; q — electron charge; ε — relative permittivity of silicon dioxide ($\varepsilon = 3.9$); ε_o — electric constant, G — the rate of generation of electron-hole pairs in case of IR, which is determined by the radiation dose rate F, the coefficient of generation of electron-hole pairs k_g and the probability of division of pairs by an electric field before their initial recombination: $G = F \cdot k_g \cdot f_y(E)$ [14].

The boundary conditions for mobile components correspond to the absorbing phase boundaries at $x = 0$ and $x = d$:

$$n(0,t) = n(d,t) = p(0,t) = p(d,t) = 0, \quad (15)$$

$$C^+_H(0,t) = C^+_H(d,t) = 0. \quad (16)$$

The gate voltage without external bias corresponds to the contact potential difference between the gate and the substrate, $V_g = \varphi$ (assumed $\varphi = 0.5\,\mathrm{V}$):

$$V(0,t) = 0, \qquad V(d,t) = \varphi. \tag{17}$$

The concentrations of all components are zero at the initial moment of time:

$$n(x,0)=p(x,0)=C^+_{TH}(x,0)=C^+_T(x,0)=C^+_H(x,0)=0, \tag{18}$$

in addition to the initial concentrations of hydrogen-containing and hydrogen-free hole traps exponentially distributed near the phase boundary (PG) Si–SiO_2:

$$C^0_{TH0}(x,0) = \frac{Q^0_{TH0}}{l}\exp\left(-\frac{x}{l}\right), \tag{19}$$

$$C^0_{T0}(x,0) = \frac{Q^0_{T0}}{l}\exp\left(-\frac{x}{l}\right), \tag{20}$$

where Q^0_{TH0} and Q^0_{T0} — initial integral concentrations (quantities) of hydrogen-containing and anhydrous traps, l — distribution width (assumed $l = 5\,\mathrm{nm}$). The shift of the threshold voltage because of the formation of a volumetric charge under the action of IR is determined by the expression

$$\Delta V_{ot} = Q_{ot}/C_{ox}, \tag{21}$$

where Q_{ot} — effective volumetric charge,

$$Q_{ot} = q\int_0^d \rho(1 - x/d)dx, \tag{22}$$

C_{ox} — dielectric specific capacitance, $C_{ox} = \varepsilon\varepsilon_0/d$, ρ — bulk charge density, $\rho = C^+_{TH} + C^+_T + C^+_H + p - n$.

We believe that a complete relaxation of the volume charge occurs when annealing is used after IR in accordance with Fig. 1:

$$TH^+ \to TH^0, \qquad T^+ \to T^0 \tag{23}$$

and the complete withdrawal of mobile hydrogen ions from the volume of the dielectric of the MOS structure:

$$C^+_H = 0 \tag{24}$$

with preserved total integral concentration of traps $(Q_{TH} + Q_T)$.

The parameters of the model are the constants of the reaction rates (1)–(6): $k_i = \sigma_{pi}V_{th}(D_p/D_n)$, $i = 1, 2, 3$; $k_{4,5} = \sigma_{n4,5}V_{th}$, $k_6 = 4\pi r_6 D^+_H$, where V_{th} — the thermal velocity of electrons ($V_{th} \cong 10^7\,\mathrm{cm/s}$), σ_p and σ_n — hole and electron capture sections (in weak fields $\sigma_p = 1.4\cdot10^{-14}\,\mathrm{cm}^2$, $\sigma_n = 1.6\cdot10^{-12}\,\mathrm{cm}^2$ [21,22]); r_6 — capture radius. We assume that $\sigma_{p2} = \sigma_{p3} = \sigma_p$, $\sigma_{n4} = \sigma_{n5} = \sigma_n$, $r_6 = 10\,\mathrm{Å}$. In addition to hole traps with a relatively large capture cross-section ($\sigma_p \cong 10^{-14}\,\mathrm{cm}^2$), centers with a smaller capture cross-section were found in thermal silicon oxide ($\sigma_p \cong 10^{-15}\,\mathrm{cm}^2$) [23]. We assume that such a capture cross section has anhydrous centers T^0, i.e. $\sigma_{p1} = 10^{-15}\,\mathrm{cm}^2$.

3. Model calculations and their discussion

Model equations (7)–(14) with boundary conditions (15)–(17), initial conditions (18)–(20), taking into account (21)–(24) were solved numerically using explicit and implicit difference schemes.

The dependence of the number of centers TH^0, TH^+, T^0 and T^+ and hydrogen ions H^+ on the number of irradiation–annealing cycles N is shown in Fig. 2. The figure shows that the number of centers TH^0 (1) and TH^+ (2) decreases after each cycle and the number of centers T^0 (3) and T^+ increases (4). This is attributable to a decrease of the number of hydrogen ions H^+ in the volume of the dielectric (5) flowing onto SiO_2-Si PB (substrate) and SiO_2-gate PB both in case of IR and especially in case of thermal annealing. That is, the TH-centers are transformed into T-centers while their total number does not change. The

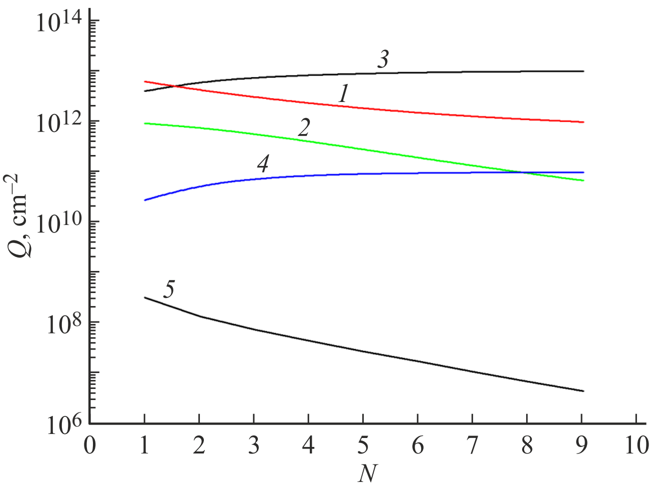

Figure 2. Effect of the number of irradiation cycles–annealing on the number of centers TH^0 (*1*), TH^+ (*2*), T_0 (*3*), T^+ (*4*) and H^+ (*5*) (model parameters are given in the caption to Fig. 3).

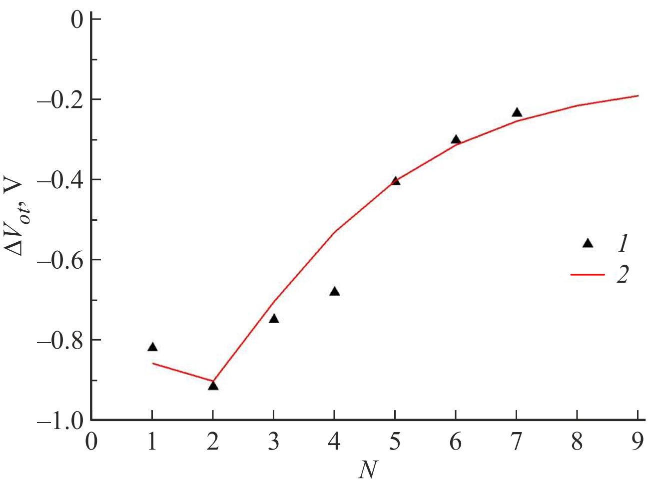

Figure 3. Dependence of the threshold voltage shift on the number of cycles irradiation–annealing: *1* — experiment, *2* — model calculation at $Q^0_{TH0} = 1.1\cdot10^{13}\,\mathrm{cm}^{-2}$, $Q^0_{T0} = 0$, $d = 120\,\mathrm{nm}$.

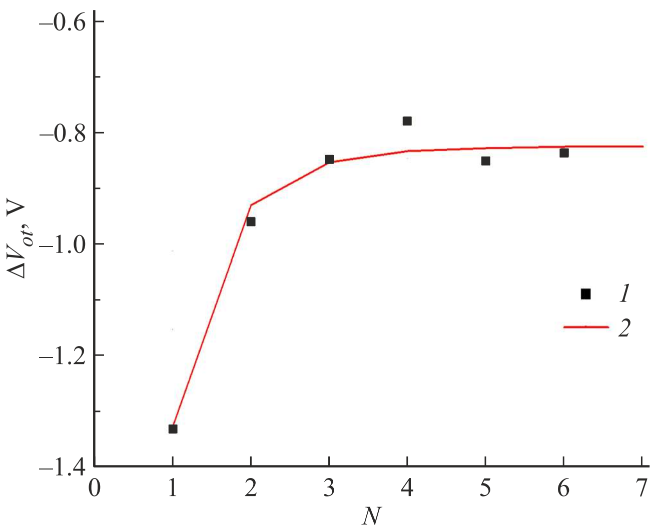

Figure 4. Dependence of the voltage shift of flat zones on the number of cycles–annealing irradiation: *1* — experiment [7], *2* — calculation by model at $Q^0_{TH0} = 8 \cdot 10^{11}\,\text{cm}^{-2}$, $Q^0_{T0} = 3.4 \cdot 10^{12}\,\text{cm}^{-2}$, $d = 35\,\text{nm}$.

number of charged T^+ centers after eight cycles becomes greater than the number of charged TH^+ centers.

The experimental dependence of the threshold voltage shift (points *1*) averaged for *n*- and *p*-MOS transistors is compared in Fig. 3 with the calculated dependence (curve *2*) at the initial the number of hydrogen-containing traps $Q^0_{TH0} = 1.1 \cdot 10^{13}\,\text{cm}^{-2}$ and with the absence of hydrogen-free traps $Q^0_{T0} = 0$. The figure shows that the increase of the number of irradiation–annealing cycles starting from the second cycle is accompanied by the reduction of the threshold voltage shift (in absolute value) during IR with a tendency for reaching a constant level. This is explained by the fact that the hydrogen released during IR by the reaction (3) goes to both phase boundaries during IR and subsequent thermal annealing, which accelerates the transformation of hydrogen-containing traps into anhydrous traps. It should be noted that the shift of the surface component of the threshold voltage is very small ($\Delta V_{it} \approx 0.06\,\text{V}$) and changes little with the increase of the number of cycles. This can be explained by the fact that the surface states completely disappear during intermediate annealing (400°C, 30 min) (i.e. they do not accumulate).

The model also allows describing the experimental data provided in Ref. [7], in which the irradiation–annealing cycles were carried out on MOS structures with an Al gate. 35 nm thick oxide was obtained by thermal oxidation at a temperature of 900°C in dry oxygen with 3% HCl. X-ray irradiation with a dose rate of 200 Krad/min was carried out for 5 min. The annealing temperature and time were 400°C and 30 min. Figure 4 shows experimental (points *1*) and calculated (curve *2*) dependences of the voltage shift of flat zones on the number of irradiation–annealing cycles with an initial number of hydrogen-containing traps $Q^0_{TH0} = 8 \cdot 10^{11}\,\text{cm}^{-2}$, and $Q^0_{T0} = 3.4 \cdot 10^{12}\,\text{cm}^{-2}$ anhydrous traps. The figure shows that the model calculation satisfactorily describes the experimental data provided in Ref. [7].

The dependence of the threshold voltage shift on the number of cycles–annealing irradiation after a certain number of cycles depending on the number of hydrogen-containing traps ($N = 7$ at $Q^0_{TH0} = 1.1 \cdot 10^{13}\,\text{cm}^{-2}$ in Fig. 3 and $N = 3$ at $Q^0_{TH0} = 8 \cdot 10^{11}\,\text{cm}^{-2}$ in Fig. 4) reaches a constant level. The relative value of the constant level is determined by the ratio of the initial concentrations of hydrogen-containing and anhydrous traps.

Conclusion

A quantitative model of the behavior of MOS structures in case of RTT has been developed. The model is based on the capture of holes formed during IR by anhydrous and hydrogen-containing traps. The capturing of holes by hydrogen-containing traps stimulates the breakage of the hydrogen bond and their transformation into anhydrous traps with a smaller capture cross section according to the model. The volumetric charge relaxes during subsequent thermal annealing, and the free hydrogen formed in the result of IR leaves the MOS structure. The model allows describing the experimental data on the increase of the radiation resistance of MOS structures during successive irradiation–annealing cycles with preserved integral concentration of traps.

Conflict of interest

The authors declare that they have no conflict of interest.

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