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Simulation of Radiation Effects in SiO_2/Si Structures

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The space–time evolution of electric charge induced in the dielectric layer of simulated metal–insulator–semiconductor structures due to irradiation with X-rays is discussed. The system of equations used as a basis for the simulation model is solved iteratively by the efficient numerical method. The obtained simulation results correlate well with the respective data presented in other scientific publications.

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1. Introduction

Currently integrated circuits (ICs) are an essential part of military and space equipment. As being used in space, such equipment is inevitably exposed to low-level ionising radiation, causing its degradation and finally malfunction. Therefore one of the urgent tasks of the microelectronics is to design and manufacture ICs with much higher radiation resistance. In this context, mathematical modelling has paramount importance by providing the solid ground for both understanding and prediction of radiation effects of X-rays in semiconductor devices. Such a simulation necessarily includes development of efficient diffusion-kinetic models and computational algorithms.

We considered the SiO_2/Si part of a simulated metal–oxide–semiconductor (MOS) structure with two types of trap levels that takes into account both the defects within the oxide layer and radiation-induced interface states. In this way we developed both physical and mathematical models of radiation-induced charge accumulation within the oxide layer and surface states due to X-ray irradiation and the subsequent charge relaxation by means of tunnel discharge. The mathematical model is basically a system of partial differential equations [1, 2] describing movement of free electrons and holes, ordinary differential equations reflecting the kinetics of charge accumulation on the hole trap levels, and the Poisson equation, which allows to compute the resulting electric field within the oxide layer. Accumulated charge in the dielectric layer discharging by the tunnelling mechanism is described by ordinary differential equations [3]. The electric field in the MOS structure in the presence of charge in the oxide layer and in surface states must adhere strictly to the principle of electroneutrality.

The model allows to describe deterioration of MOS structures caused by ionising radiation. Deterioration onset influences threshold voltage specific to the structure. The fluence dependence of the threshold voltage is determined by depth distribution of traps and mobility and capture cross-sections for electrons and holes.

The numerical solution is based on the difference method [4]. The developed iterative algorithm allows us to simulate the following properties of the MOS structure: radiation-induced changes of the threshold voltage as a function of radiation dose, electric charge distribution in the oxide layer with various thickness, the resulting effective charge and electric field within the MOS structure during irradiation, etc.

2. The model

The following system of equations describes the radiation dynamics of electric charge distribution [1–3] in the dielectric layer with the thickness d of metal–insulator–semiconductor (MIS) structure shown in Fig. 1. These equations take into account tunnelling discharge as well. The solution has to be found within the area $\Omega = \{0 < x < d, 0 < t < t_j\}$, where t_j is a simulation time

$$\frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} + \mu_n \frac{\partial (nE)}{\partial x} - R_{n1}(n, E, P_{t1}) - R_{n2}(n, E, P_{t2}) + G(E), \tag{1}$$

$$\frac{\partial p}{\partial t} = D_p \frac{\partial^2 p}{\partial x^2} + \mu_p \frac{\partial (pE)}{\partial x} - R_{p1}(p, E, P_{t1}) - R_{p2}(p, E, P_{t2}) + G(E), \tag{2}$$

$$\frac{\partial P_{t1}}{\partial t} = R_{p1}(p, E, P_{t1}) - R_{n1}(n, E, P_{t1}),$$
$$\frac{\partial P_{t2}}{\partial t} = R_{p2}(p, E, P_{t2}) - R_{n2}(n, E, P_{t2}), \tag{3}$$

$$\frac{\partial E}{\partial x} = \frac{q}{\varepsilon_{0x}\varepsilon_0} \left(P_{t1} + P_{t2} + p - n\right), \tag{4}$$

$$\frac{\partial P_t}{\partial t} = -\alpha_1 \exp(-\alpha_2 x) P_t, \tag{5}$$

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$$V_{\mathrm{g}} = \phi_{ms} + \psi - \left(\frac{Q_{0t}}{C_{ox}} + \frac{Q_{sc}(\psi)}{C_{ox}} + \frac{Q_{ss}(\psi)}{C_{ox}}\right). \qquad (6)$$

The respective initial and boundary conditions are as follows:

$$n(0,t) = n(d,t) = 0,$$

$$p(0,t) = p(d,t) = 0,$$

$$0 < t \le t_f;$$

$$Q_{0t}(0) = Q_{ss}(0) = 0;$$

$$n(x,0) = p(x,0) = P_{t1}(x,0) = P_{t2}(x,0) = 0,$$

$$E(x,0) = f(\psi(0)),$$

$$0 \le x \le d. \qquad (7)$$

Equations (1)–(7) contain the following parameters: n, p stand for the concentration of free electrons and holes, E is the electric field, P_{t1} is the concentration of holes captured on the shallow trap levels (both oxide–gate and oxide–semiconductor interfaces), P_{t2} is the concentration of holes captured on the deep trap levels (inside the oxide layer), D_n, D_p are the diffusion coefficients of electrons and holes, μ_n, μ_p are mobilities of electrons and holes, G is the generation rate of the electron–hole pairs due to ionising radiation, q is the electron charge, ε is the dielectric permittivity of SiO_2, $R_{n1,2}$, $R_{p1,2}$ are the capture rates of electrons and holes on the shallow and deep trap levels, V_{g} is the gate voltage, φ_{ms} is the difference of the work functions of the gate and semiconductor materials, ψ is the surface potential of semiconductor, α_1, α_2 are the frequency and barrier factors, C_{ox} is the dielectric layer capacity, Q_{ss} is the surface state charge, Q_{sc} is charge of the space-charge region of the semiconductor, Q_{0t} is the effective charge captured on the trap levels in the SiO_2 layer.

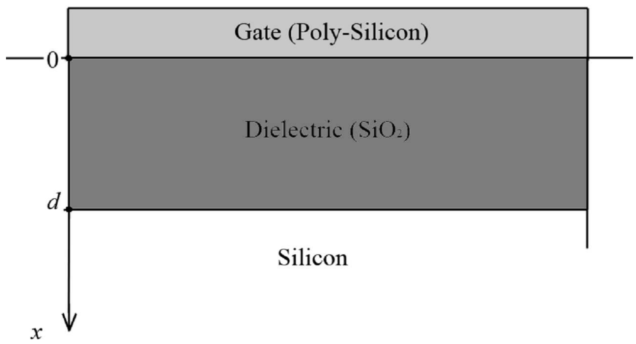

Fig. 1. The model of MIS structure.

The model is complemented by the following equations. Capture rates of electrons and holes on the trap levels are defined as in Ref. [1]:

$$R_{n1} = nP_{t1}\sigma_n(E)\left(\mu_n |E| + v_{th}\right),$$

$$R_{n2} = nP_{t2}\sigma_n(E)\left(\mu_n |E| + v_{th}\right),$$

$$R_{p1} = p\left(N_{t1} - P_{t1}\right)\sigma_p(E)\left(\mu_p |E| + \frac{\mu_p}{\mu_n} v_{th}\right),$$

$$R_{p2} = p\left(N_{t2} - P_{t2}\right)\sigma_p(E)\left(\mu_p |E| + \frac{\mu_p}{\mu_n} v_{th}\right), \qquad (8)$$

where $N_{t1,2}(x)$ are the concentrations of hole traps, v_{th} is the thermal velocity of charge carriers, $\sigma_p(E)$ and $\sigma_n(E)$ are the capture cross-sections for holes and electrons, respectively.

The generation rate of electron–hole pairs $G(E)$ depends on the radiation dose intensity $\dot{\mathrm{D}} = \mathrm{d}D/\mathrm{d}t$, pairs generation coefficient k_{g} and the probability for the created electron–hole pairs to be separated by the electric field before recombination $f_y^{\mathrm{X-ray}}(E)$ [5, 6]:

$$G(E) = \dot{\mathrm{D}} k_{\mathrm{g}} f_y^{\mathrm{X-ray}}(E).$$

The electric charge in the bulk of the oxide layer and at the interfaces

$$Q_{0t} = \frac{1}{d}\int_0^d (d-x)\rho_t(x)\,\mathrm{d}x$$

and

$$Q_{ss} = qN_{ss}(\varphi_0 - \psi), \qquad (9)$$

where $\rho_t(x)$ is the distribution of hole charge accumulated on the trap levels, $N_{ss} = k_{\mathrm{D}} Q_{0t}/q/\varphi_0$ is the surface state density [7, 8] averaged to the band gap energy (k_{D} is determined experimentally).

Charge of the space-charge region is calculated as in [9]:

$$Q_{sc}(\psi) = \varepsilon_s\varepsilon_0 E_s = \pm\frac{\sqrt{2}\varepsilon_s\varepsilon_0 kT}{qL_{\mathrm{D}}} F(\psi, \phi_0). \qquad (10)$$

3. The modified system of equations

Taking into account Eqs. (8), the system (1)–(10) can be written in the following form:

$$\frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} + \mu_n \frac{\partial\,(nE)}{\partial x}$$
$$-nQ_1(E, P_{t1}, P_{t2}) + G(E), \qquad (11)$$

$$\frac{\partial p}{\partial t} = D_p \frac{\partial^2 p}{\partial x^2} + \mu_p \frac{\partial\,(pE)}{\partial x}$$
$$-pQ_2(E, P_{t1}, P_{t2}) + G(E), \qquad (12)$$

$$\frac{\partial P_{t1}}{\partial t} = -P_{t1}S_1(p,n,E) + S_2(p,E)N_{t1},$$

$$\frac{\partial P_{t2}}{\partial t} = -P_{t2}\,S_1(p,n,E) + S_2(p,E)N_{t2}, \qquad (13)$$

$$\frac{\partial E}{\partial x} = \frac{q}{\varepsilon_{0x}\varepsilon_0}\left(P_{t1} + P_{t2} + p - n\right), \qquad (14)$$

$$\frac{\partial P_t}{\partial t} = -P_t S_3(E), \qquad (15)$$

$$-V_{\mathrm{g}} + \phi_{ms} + \psi - \left(\frac{Q_{0t}}{C_{ox}} + \frac{Q_{sc}(\psi)}{C_{ox}} + \frac{Q_{ss}(\psi)}{C_{ox}}\right)$$
$$= 0, \qquad (16)$$

where

$$Q_1(E, P_{t1}, P_{t2}) = (P_{t1} + P_{t2})\sigma_n(E)\left(\mu_n |E| + v_{th}\right),$$

$$Q_2(E,P_{t1},P_{t2}) = (N_{t1} - P_{t1} + N_{t2} - P_{t2})\,\sigma_p(E) \times \left(\mu_p\,|E| + \frac{\mu_p}{\mu_n} v_{th}\right).$$

$$S_1(p,n,E) = p\sigma_p(E)\left(\mu_p\,|E| + \frac{\mu_p}{\mu_n} v_{th}\right) + n\sigma_n\left(\mu_n\,|E| + v_{th}\right),$$

$$S_2(p,E) = p\sigma_p(E)\left(\mu_p\,|E| + \frac{\mu_p}{\mu_n} v_{th}\right),$$

$$S_3(E) = \alpha_1(E)\exp(-\alpha_2 x).$$

4. The algorithm

The solution of the system of Eqs. (11)–(16) with boundary conditions (7) is based on iteration algorithm. Each time step $t = t_j$ includes the following stages:
(a) First, the initial-boundary value problem for the continuity Eq. (11) together with the initial and boundary conditions (7) is solved in order to calculate the depth distribution of free electrons $n(x,t_j)$.
(b) Next by taking into account the results obtained in the previous stage and by solving the initial-boundary value problem for the continuity Eq. (12), one can calculate the depth distribution of holes $p(x,t_j)$.
(c) Further, the calculated distributions of free charge carriers $n(x,t_j)$ and $p(x,t_j)$ are put into Eq. (13) describing capture kinetics of holes. In this way the spatial distribution of hole charge accumulated on the trap levels $P_{t1}(x,t_j)$ and $P_{t2}(x,t_j)$ is determined.
(d) Then Eq. (15) is solved in order to take into account the tunnel discharging of captured charge in the dielectric layer.
(e) Next the depth distributions of free electrons $n(x,t_j)$, free holes $p(x,t_j)$, and captured charge $P_{t1}(x,t_j)$ and $P_{t2}(x,t_j)$ found in the previous stages are put into the Poisson Eq. (14) thus allowing to compute the electric field in the oxide layer.
(f) Using the results of all the previous stages, one can solve the equation of electroneutrality (16) defining many properties of the MOS structure as a whole and calculate the value of the surface potential of the semiconductor $\psi(t_j) = \overset{s+1}{\psi}$, where $s = 0,\ 1,\ 2$ is the iteration number.
(g) The termination condition for the time step $t = t_j$ is $\left|\overset{s+1}{\psi} - \overset{s}{\psi}\right| \le \varepsilon_1 \left|\overset{s}{\psi}\right| + \varepsilon_2$, $\varepsilon_1, \varepsilon_2$ are the empirical constants ($\varepsilon_1 = 0$ if $\left|\overset{s}{\psi}\right| < 1$ and $\varepsilon_2 = 0$ if $\left|\overset{s}{\psi}\right| > 1$). If the indicated termination condition is fulfilled, we calculate the threshold voltage, the effective charge in the oxide layer and other characteristics of MOS-structure at time t_j. Otherwise, we first use the obtained distribution $E(x,t_j)$ to recalculate the functions $n(x,t_j), p(x,t_j)$, $R_{t1}(x,t_j)$ and $R_{t2}(x,t_j)$. Finally, we increment time and thus proceed to the next time step going again through the stages (a)–(g) mentioned above.

The presented algorithm is applied numerically. The developed numerical method is based on the difference method [4]. The difference problem is solved iteratively. The numerical solution of the initial-boundary problems for the continuity equations $n(x,t_j), p(x,t_j)$ is obtained by the sweep method [4]. The electro-neutrality Eq. (16) is solved by means of the bisection method.

5. Results

The numerical simulations of radiation-induced changes in the threshold voltage of the MOS structures due to 20 keV X-rays have been performed. Some results of simulation are presented in Figs. 1–3. The calculations were done with the following values: the radiation dose of X-rays $D = 5 \times 10^5$ R with the intensity $\dot{D} = dD/dt = 10^2$ R/s, impurity concentration in silicon $N_B = 10^{15}$ cm^{-3}, temperature $T = 300$ K, $\varphi_{ms} = -0.5$ V, the mobility of electrons $\mu_n = 10^2$ cm^2 V^{-1} s^{-1} and holes $\mu_p = 0.6\times10^{-3}$ cm^2 V^{-1} s^{-1} in the oxide layer. The generation rate of the electron–hole pairs in SiO_2 is $k_g = 8 \times 10^{12}$ cm^{-3} rad^{-1} pairs [10], the permittivity values are $\varepsilon_{ox} = 1.6$ and $\varepsilon_s = 11.5$.

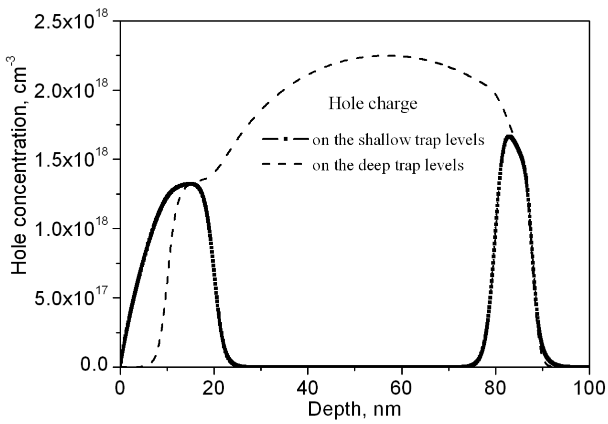

Fig. 2. Depth distribution of holes on the trap levels after the irradiation.

Figure 2 shows the calculated depth distribution of holes bound by both "shallow" and "deep" trap levels in the SiO_2 layer with the thickness d of 100 nm. The calculations were made for $V_G = -0.9$ V, $k_D = 1.03$ and the distribution of "shallow" N_{t1} and "deep" N_{t2} trap levels [1]:

$$N_{t1} = 5 \times 10^{18}\left[\left(e^{(x-20)} + 1\right)^{-1} + \left(e^{(80-x)} + 1\right)^{-1}\right],$$

$$N_{t2} = 5 \times 10^{18}\left[\left(e^{(x-90)} + 1\right)^{-1} - \left(e^{(x-10)} + 1\right)^{-1}\right].$$

Figures 3 and 4 show the results of simulation for $V_G = -1$ V, $k_D = 1.15$, $N_{t1} = 5 \times 10^{18}$ cm^{-3}, and $N_{t2} = 10^{19}$ cm^{-3}. Figure 2 shows the change in the threshold voltage of the simulated MOS structure due to its irradiation with X-rays. The calculations were made

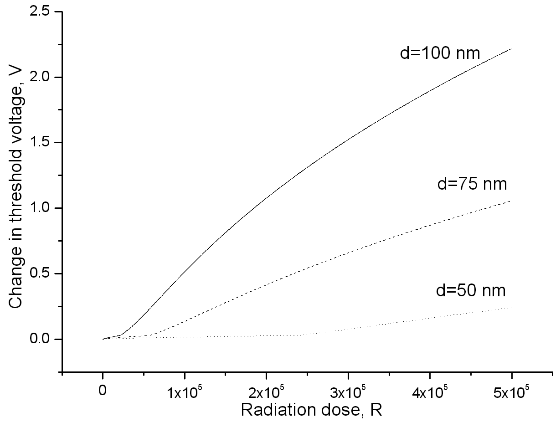

Fig. 3. Radiation-induced change in the threshold voltage for variously thick SiO_2 layer within the MOS structure.

for three values of SiO_2 layer thickness. One can see that the thinner the oxide layer, the lower is the respective radiation effect on the threshold voltage and thus the higher is the radiation resistance. For example, the simulated MOS structure with a 50 nm thick SiO_2 layer is much more radiation-resistant than that with a 100 nm thick SiO_2layer (see Fig. 3). This is due to lower concentration of accumulated hole charge in oxide as well as its distribution to "shallow" and "deep" trap levels. Figure 4 illustrates the depth distribution of holes bound on "shallow" and "deep" trap levels in SiO_2 for various thickness of the oxide layer. The obtained simulation results correlate well with the data in Refs. [1, 11, 12].

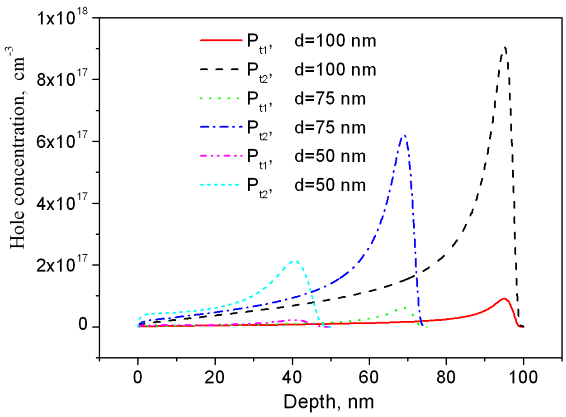

Fig. 4. Depth distribution of bound holes in the SiO_2 layer with various thickness.

6. Conclusion

The offered model can be used to simulate radiation-induced deterioration of MOS structures and to calculate the radiation-induced changes in the MOS threshold voltage depending on the depth distribution of the traps within the silicon oxide layer and on the mobility and capture cross-sections of electrons and holes. Furthermore, also depth distributions of free and bound/trapped electrons and holes in the SiO_2 layer, the resulting electric field intensity, and the change of surface potential of the oxide–semiconductor interface in the MOS structure can be computed as well. The obtained simulation results correlate well with the experimental data.

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