PROCEEDINGS OF THE INTERNATIONAL CONFERENCE
NANOMATERIALS: APPLICATIONS AND PROPERTIES
Vol. **3** No 1, 01PISERE04(4pp) (2014)

Simulation of Radiation Effects in SiO_2/Si Structures

A.F. Komarov[1,*], G.M. Zayats[2,†], F.F. Komarov[1], S.A. Miskiewicz[1], V.V. Michailov[1]

[1] *Institute of Applied Physics Problems, 7, Kurchatov Str., 220045 Minsk, Belarus*
[2] *Institute of Mathematics, National Academy of Sciences of Belarus, 11, Surganov Str., 220072 Minsk, Belarus*

(Received 31 July 2014; published online 29 August 2014)

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

Keywords: Integrated circuits, Radiation, MIS, Numerical iimulation.

PACS numbers: 02.30.Hq, 02.60.Cb

1. INTRODUCTION

Currently, integrated circuits (IC) are 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 solid ground for both understanding and prediction of radiation effects of X-rays in semiconductor devices.

We considered the SiO2/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 irradiation with X-rays and the subsequent charge relaxation by means of tunnel discharge. The mathematical model is basically a system of partial differential Eq. [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 resulting electric field within the oxide layer. Accumulated charge in the dielectric layer discharging by the tunnelling mechanism is described by ordinary differential Eq. [3].

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 by mobility and capture cross sections for electrons and holes.

The numerical solution is based on the difference method [4]. The developed iterative algorithm allowed 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 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 thickness *d* of MIS shown on Fig. 1. These equations take into account tunnelling discharge as well. The solution has thus to be found within the area $\Omega=\{0<x<d,\ 0<t<t_j\}$, where t_j is a simulation time.

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

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

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

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

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

$$V_G=\varphi_{ms}+\psi-\left(\frac{Q_{0t}}{C_{ox}}+\frac{Q_{sc}(\psi)}{C_{ox}}+\frac{Q_{ss}(\psi)}{C_{ox}}\right) \quad (6)$$

The respective initial and boundary conditions are as follows:

$$\begin{aligned}&n(0,t)=n(d,t)=0,\\ &p(0,t)=p(d,t)=0,\\ &0<t\le t_f;\\ &Q_{0t}(0)=Q_{ss}(0)=0;\\ &n(x,0)=p(x,0)=P_{t1}(x,0)=P_{t2}(x,0)=0,\\ &E(x,0)=f(\psi(0)),\\ &0\le x\le d.\end{aligned} \quad (7)$$

The Eqs. (1) – (7) contains the following parameters: *n, p* stand for concentration of free electrons and holes, *E* is electric field, P_{t1} is concentration of holes

---

[*] koma-rovf@bsu.by
[†] zayats@im.bas-net.by

captured on the shallow trap levels (both oxide-gate and oxide-semiconductor interfaces), P_{t2} is concentration of holes captured on the deep trap levels (inside the oxide layer), D_n, D_p are diffusion coefficients of electrons and holes, μ_n, μ_p are mobilities of electrons and holes, G is generation rate of the electron-hole pairs due to ionising radiation, q is electron charge, ε is dielectric permittivity of SiO_2, $R_{n1,2}$, $R_{p1,2}$ are capture rates of electrons and holes on the shallow and deep trap levels, V_G is gate voltage, φ_{ms} is difference of the work functions of the gate and semiconductor materials, ψ is surface potential of semiconductor, α_1, α_2 are frequency and barrier factors, C_{ox} is dielectric layer capacity, Q_{ss} is 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 SiO_2 layer.

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

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

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

$$R_{p1} = p\left(N_{t1} - P_{t1}\right)\sigma_p(E)\left(\mu_p|E| + \frac{\mu_p}{\mu_n}v_{th}\right), \qquad (8)$$

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

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

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

$$G(E) = \dot{D}k_g f_y^{x-ray}(E)\,.$$

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

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

and

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

where $\rho_t(x)$ is distribution of hole charge accumulated on the trap levels, $N_{ss}=k_D Q_{0t}/q/\varphi_0$ 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]

$$Q_{sc}(\psi) = \varepsilon_s\varepsilon_0 E_s = \pm\frac{\sqrt{2}\varepsilon_s\varepsilon_0 kT}{qL_D}F(\psi,\varphi_0) \qquad (10)$$

3. THE MODIFIED SYSTEM OF EQUATION

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

$$\frac{\partial n}{\partial t} = D_n\frac{\partial^2 n}{\partial x^2} + \mu_n\frac{\partial(n\cdot E)}{\partial x} - n\,Q_1(E,P_{t1},P_{t2}) + G(E), \quad (11)$$

$$\frac{\partial p}{\partial t} = D_p\frac{\partial^2 p}{\partial x^2} + \mu_p\frac{\partial(p\cdot E)}{\partial x} - p\,Q_2(E,P_{t1},P_{t2}) + G(E), \quad (12)$$

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

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

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

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

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

where

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

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

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

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

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

4. 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 $D = 5\cdot10^5$ R with intensity $\dot{D} = dD/dt = 10^2$ R/s, impurity concentration in silicon $N_B = 10^{15}$ cm^{-3}, temperature T = 300K, φ_{ms}=-0.5V, the mobility of electrons $\mu_n = 10^2$cm^{2}V^{-1}s^{-1} and holes μ_p=0.6$\cdot10^{-3}$ cm^{2}V^{-1}s^{-1} in oxide layer. The generation rate of electron-hole pairs in SiO_2 is k_g=8x10^{12} cm^{-3}rad^{-1} pairs [10], the permittivity values are ε_{ox}=1.6 and ε_s=11.5.

Fig. 2 shows the calculated depth distribution of holes bound by both “shallow” and “deep” trap levels in

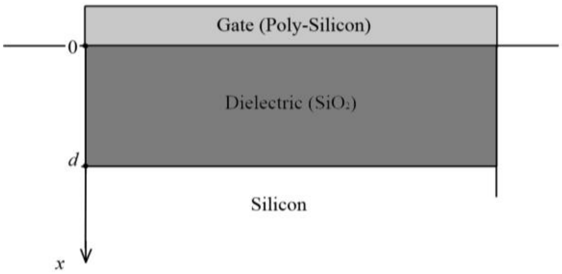

Fig. 1 – The model of MIS structure.

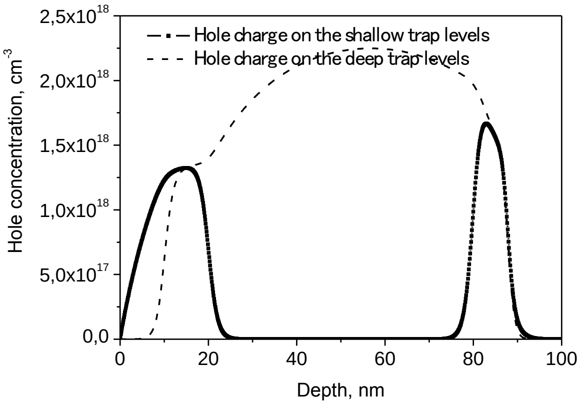

Fig. 2 – Depth distribution of holes on the trap levels after the irradiation

the SiO$_2$ layer with thickness d of 100 nm. The calculations were made for V_G=-0.9V, k_D=1.03 and the distribution of "shallow" N_{t1} and "deep" N_{t2} trap levels [1]:

$$N_{t1} = 5\times10^{18}\left(\left(e^{(x-20)}+1\right)^{-1}+\left(e^{(80-x)}+1\right)^{-1}\right),$$

$$N_{t2} = 5\times10^{18}\left(\left(e^{(x-90)}+1\right)^{-1}-\left(e^{(x-10)}+1\right)^{-1}\right).$$

Figs. 3 and 4 show the results of simulation for V_G = -1 V, k_D =1.15, N_{t1}=5x10^{18} cm^{-3}, and N_{t2}=10^{19} cm^{-3}. Fig. 2 shows the change in threshold voltage of the simulated MOS structure due to its irradiation with X-rays. The calculations have been performed 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$_2$ layer (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. Fig. 4 illustrates 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 data in Refs. [1, 11, 12].

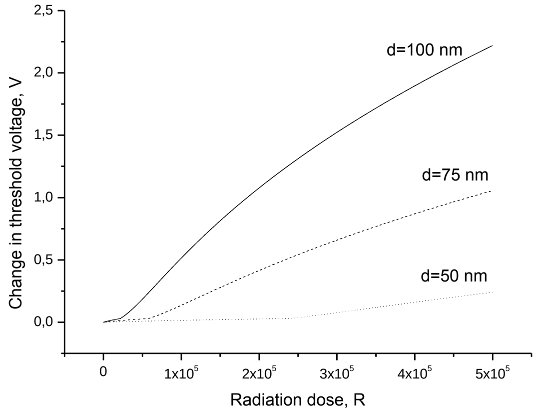

Fig. 3 – The radiation-induced change in threshold voltage for variously thick SiO$_2$ layer within MOS structure.

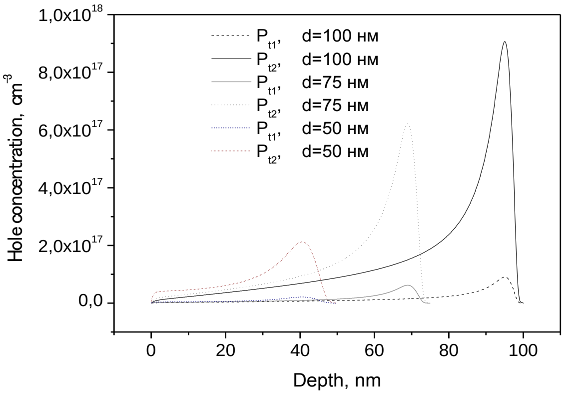

Fig. 4 – Depth distribution of bound holes in SiO$_2$ layer with various thickness.

5. 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 SiO$_2$ layer, the resulting electric field intensity, and the change of surface potential of the oxide-semiconductor interface in MOS structure can be computed as well. The obtained simulation results correlate well with experimental data.

REFERENCES

1. M.N. Levin, A.V. Tatarintsev, V.A. Makarenko, V.R. Gitlin, *Microelectronics* **35**, 382 (2006).
2. G.M. Zayats, A.F. Komarov, F.F. Komarov, S.A. Miskiewicz, *Reports of NAS of Belarus* **57**, 53 (2013).
3. P.J. MCWhorter, S.L. Miller, W.M. Miller, *IEEE T. Nucl. Phys.* **37**, 1682 (1990).
4. A.A. Samarskij, *Theory of Difference Schemes*, (Nauka: Moscow: 1989).

5. G.A. Ausman, F.B. McLean, *Appl. Phys. Lett.* **26**, 173 (1975).
6. J.M. Benedetto, H.E. Boesch, *IEEE T. Nucl. Sci.* **6**, 1318 (1986).
7. A.G. Kadmenskij, S.G. Kadmenskij, M.N. Levin, V.M. Maslovskij, V.E. Chernyshev, *Tech. Phys. Lett.* **19** (1993).
8. M.N. Levin, V.M. Maslovsky, *Solid State Comm.* **90**, 813 (1994).
9. V.A. Gurtov, *Solid-state Electronics: Tutorial* (Petrozavodsk: 2004).
10. A.V. Sogojan, *Spase Model: in 2 v.* (Moscow State University, Institut of Nuclear Physics, Moscow: 2007).
11. M.N. Levin, *Condenced matters and phase interfaces* 12, 226 (2010).
12. E.V. Bondarenko, *Simulation of Low-Level Radiation Impact on the Mischarge Properties* (Voronezh: 2010).