Simulation of Radiation Effects in SiO₂/Si Structures

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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 simulation.

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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 ionizing 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 ionizing 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 Ω={0<x<d, 0<t<t₁}, where t₁ is a simulation time.

\[
\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} + \mu_e \frac{\partial (nE)}{\partial x} - R_{11}(n, E, P_{11}) - R_{21}(n, E, P_{21}) + G(t,E),
\]

\[
\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2} + \mu_h \frac{\partial (pE)}{\partial x} - R_{21}(p, E, P_{21}) - R_{12}(p, E, P_{12}) + G(t,E),
\]

\[
\frac{\partial P_{11}}{\partial t} = R_{11}(p, E, P_{11}) - R_{11}(n, E, P_{11}),
\]

\[
\frac{\partial P_{22}}{\partial t} = R_{22}(p, E, P_{22}) - R_{22}(n, E, P_{22}),
\]

\[
\frac{\partial E}{\partial x} = \frac{q}{\varepsilon_0}(P_{11} + P_{22} + p - n)
\]

\[
\frac{\partial P_t}{\partial t} = -\alpha_c \exp(-\alpha_c x) P_t
\]

\[
V_O = q_{ox} + \psi - \left( \frac{Q_{ox}}{C_{ox}} + \frac{Q_0(\psi)}{C_{ox}} \right)
\]

The respective initial and boundary conditions are as follows:

\[
n(0,t) = n(d,t) = 0,
\]

\[
p(0,t) = p(d,t) = 0,
\]

\[
0 < t < t₁ ;
\]

\[
Q_{ox}(0) = Q_{ox}(d) = 0 ;
\]

\[
n(x,0) = p(x,0) = P_{11}(x,0) = P_{22}(x,0) = 0,
\]

\[
E(x,0) = f(\psi(0)),
\]

\[
0 < x < d .
\]

The Eqs. (1) – (7) contains the following parameters: n, p stand for concentration of free electrons and holes, E is electric field, P₁₁ is concentration of holes

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captured on the shallow trap levels (both oxide-gate and oxide-semiconductor interfaces), \( P_2 \) 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, \( \mu_n, \mu_p \) are mobilities of electrons and holes, \( G \) is generation rate of the electron-hole pairs due to ionising radiation, \( q \) is electron charge, \( v \) is dielectric permittivity of SiO\(_2\), \( R_{0.1,2}, R_{0.1,2} \) are capture rates of electrons and holes on the shallow and deep trap levels, \( V_G \) is gate voltage, \( \varphi_{so} \) is difference of the work functions of the gate and semiconductor materials, \( \psi \) is surface potential of semiconductor, \( \alpha_1, \alpha_2 \) are frequency and barrier factors, \( C_{so} \) is dielectric layer capacity, \( Q_{so} \) is surface state charge, \( Q_{so} \) is charge of the space-charge region of the semiconductor, \( Q_{so} \) 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]

\[
R_{n1} = n_p \sigma_n(E)(\mu_n[E] + v_n) \\
R_{n2} = n_p \sigma_n(E)(\mu_n[E] + v_n) \\
R_{p1} = p(N_{11} - P_{11}) \sigma_p(E)(\mu_p[E] + \mu_p v_n) \\
R_{p2} = p(N_{12} - P_{12}) \sigma_p(E)(\mu_p[E] + \mu_p v_n) \\
\text{where } N_{11,2}(x) \text{ are concentrations of hole traps; } v_n \text{ is the thermal velocity of charge carriers; } \alpha_n(E) \text{ and } \alpha_o(E) \text{ are capture cross-sections for holes and electrons, respectively.}
\]

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

\[
G(E) = D k_g f^{xos}(E)
\]

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

\[
Q_{so} = \frac{1}{d} \int_{0}^{d}(d - x)p(x)dx \\
\text{and } \\
Q_{so} = qN_{so}(\varphi_0 - \psi) \\
\text{where } p(x) \text{ is distribution of hole charge accumulated on the trap levels, } N_{so} = k_qQ_{so}/q \text{ is the surface state density [7, 8] averaged to the band gap energy (} k_q \text{ is determined experimentally).}
\]

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

\[
Q_{so}(\psi) = e_qN_{so}E_0 = \pm \sqrt{\frac{2e_q\varphi_{so}kT}{qL_D}} F(\psi, \varphi_0) \quad (10)
\]

3. **THE MODIFIED SYSTEM OF EQUATION**

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

\[
\frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} + \mu_n \frac{\partial (n - E)}{\partial x} - n Q(E, P_{11}, P_{21}) + G(E), \quad (11)
\]

\[
\frac{\partial p}{\partial t} = D_p \frac{\partial^2 p}{\partial x^2} + \mu_p \frac{\partial (p - E)}{\partial x} - p Q(E, P_{11}, P_{21}) + G(E), \quad (12)
\]

\[
\frac{\partial n}{\partial t} = -P_nS_1(n, E) + S_2(p, E)N_{so}, \quad (13)
\]

\[
\frac{\partial p}{\partial t} = -P_pS_1(n, E) + S_2(p, E)N_{so}, \quad (14)
\]

\[
\frac{\partial E}{\partial x} = \frac{q}{\varepsilon_{so}} (P_{11} + P_{21} + p - n), \quad (15)
\]

\[
-V_G + \varphi_0 + \psi - \frac{Q_{so}}{C_{so}} - \frac{Q_{so}(\psi)}{C_{so}} = 0, \quad (16)
\]

where

\[
Q(E, P_{11}, P_{21}) = (N_{11} - P_{11} + N_{12} - P_{12}) \sigma_p(E)(\mu_p[E] + \mu_p v_n) \\
S_1(n, E) = p\sigma_p(E)(\mu_p[E] + \mu_p v_n) + n\sigma_n(\mu_n[E] + v_n) \\
S_2(p, E) = p\sigma_p(E)(\mu_p[E] + \mu_p v_n), \quad (17)
\]

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 \( D = 5 \times 10^8 \text{R} \) with intensity \( D = dD/dt = 10^2 \text{ R/s} \), impurity concentration in silicon \( N_0 = 10^{15} \text{ cm}^{-3} \), temperature \( T = 300 \text{K} \), \( \varphi_{so} = 0.5 \text{V} \), the mobility of electrons \( \mu_n = 10^3 \text{ cm}^2/\text{V} \cdot \text{s} \) and holes \( \mu_p = 10^{-3} \text{ cm}^2/\text{V} \cdot \text{s} \) in oxide layer. The generation rate of electron-hole pairs in SiO\(_2\) is \( k_o = 8 \times 10^5 \text{ cm}^2/\text{rad} \cdot \text{s} \) pairs [10], the permittivity values are \( \varepsilon_{so} = 1.6 \) and \( \varepsilon_{si} = 11.5 \).

Fig. 2 shows the calculated depth distribution of holes bound by both “shallow” and “deep” trap levels in
The SiO₂ layer with thickness \( d \) of 100 nm. The calculations were made for \( V_0 = -0.9 \text{V}, \) \( k_B = 1.03 \) and the distribution of “shallow” \( N_{t1} \) and “deep” \( N_{t2} \) trap levels \([1]\):

\[
N_{t1} = 5 \times 10^{18} \left( e^{(x-20)} + 1 \right)^{-1} \left( e^{(x-90)} + 1 \right)^{-1},
\]

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

Figs. 3 and 4 show the results of simulation for \( V_0 = -1 \text{V}, \) \( k_B = 1.15, \) \( N_{t1} = 5 \times 10^{18} \text{ cm}^{-3} \), and \( N_{t2} = 10^{19} \text{ cm}^{-3} \). 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 SiO₂ 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 SiO₂ layer is much more radiation-resistant than that with a 100 nm thick SiO₂ 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 SiO₂ for various thickness of the oxide layer. The obtained simulation results correlate well with data in Refs. \([1, 11, 12]\).

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 SiO₂ 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.

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