Semiconductors, 2022, Vol. 56, No. 12

Dispersive transport of Hole polarons in MOS-structures after the ionizing irradiation

© *O.V. Aleksandrov*

St. Petersburg State Electrotechnical University „LETI“,
197376 St. Petersburg, Russia

E-mail: Aleksandr_ov@mail.ru

Received July 20, 2022
Revised November 22, 2022
Accepted December 18, 2022

It is shown that the description of the dispersive transport of hole polarons based on the multiple capture model makes it possible to quantitatively describe the kinetics of the accumulation and relaxation of space charge in MOS-structures after ionizing irradiation at low temperatures (80−293 K). Modeling of time dependences of threshold voltage on temperature, electric field strength and gate oxide thickness is carried out. It is shown that the kinetics of space charge relaxation is determined by the hopping transport of hole polarons with the levels of localized states in the range of 0.08−0.55 eV, the concentration of polaron states, the influence of the electric field strength on the average polaron energy, as well as gate oxide thickness on dispersive parameter. The polaron radius is estimated.

Keywords: MOS-structure, the ionizing radiation, dispersive transport, polarons, modeling.

DOI: 10.21883/SC.2022.12.55153.3947

1. Introduction

A positive space charge (SC) in a gate insulator and surface states (SS) at the Si−SiO$_2$ interphase boundary (IPB), which affect the electric parameters of devices, are produced in the process of ionizing irradiation (IIR) of MOS structures [1–3]. The accumulation of SC in an insulator and its subsequent relaxation at low irradiation temperatures ($T < 300$ K) are attributable to the low mobility of holes in silicon dioxide SiO$_2$ [4–6]. The relaxation of hole SC after pulsed IIR is completed within a fraction of a second at room temperature, but may extend over several hours at lower temperatures [4–6]. The authors of [4,7] attributed this effect to the formation of hole polarons (a combination of a hole and the elastic field produced by it) and their hopping transport over localized states in the bandgap of amorphous SiO$_2$. Hole polarons move in the disordered structure of amorphous SiO$_2$ by hopping between potential wells of a varying depth (localized states), which entrap them for a certain time that depends on the depth. This dispersive transport was characterized in [4–7] with the use of the continuous time random walk (CTRW) model developed by Scher and Montrol [8]. The CTRW model was used to determine the dependences of the flat-band voltage [4–6] and the relative current density [7] in MOS structures on time elapsed after an IIR pulse. It was demonstrated that the experimental data fit in with a universal curve representing the dependence of the measured quantity (normalized to its maximum value) on the logarithm of time normalized to the time of dependence slope break. Dispersion parameter α was determined based on the slope of dependences ($0 < \alpha < 1$). It was found that α is independent of IIR temperature [7], but depends on the method of fabrication of MOS structures and falls within the range of 0.14−0.3 [4,7]. Note that the CTRW theory allows one to characterize only the shape of a temporal dependence of a relative measured quantity.

The process of dispersive transport of charge carriers in disordered materials may also be characterized using the model of multiple trapping (MT) of carriers by localized states (traps) with a range of binding energies [9]. The equivalence of MT and CTRW models was established in [9,10]. Characterizing the dispersive transport of holes in SiO$_2$, the authors of [11] demonstrated that the MT model has several advantages over CTRW. Specifically, it provides a closer fit to experimental data on the accumulation of hole charge over short and long scales of time elapsed after IIR at various temperatures and electric field strengths [11]. In addition, the MT model was found to provide a quantitative description of dispersive transport in the case of H in SiO$_2$ (see [12]).

The aim of the present study is to characterize quantitatively and analyze the dispersive transport of hole polarons in gate SiO$_2$ after low-temperature ionizing irradiation of MOS structures using the model of multiple trapping.

2. Description of the model

In contrast to crystalline solids, amorphous solids have no long-range ordering, featuring only short-range order. The Si−O−Si bridge bond angles in the network of amorphous silicon dioxide SiO$_2$ vary from 120 to 180° [19], thus inducing a spread (dispersion) of energies of binding between a hole polaron and network atoms. The polaron hole transport in amorphous SiO$_2$ is effected by hopping, as was assumed in [7], over $2p_\pi(O)$ oxygen orbitals or, as was demonstrated in [13], over $3s$, $3p$, $3d\,(\mathrm{Si})-2p$, $2s\,(\mathrm{O})$ orbitals (i.e., closely adjacent Si and O atoms). We regard potential wells for hole polarons in SiO$_2$ as localized states.

In accordance with the model of multiple trapping, we substitute a continuous energy distribution of localized states by a system of k states with discrete levels E_{bi} corresponding to the energy of ith localized states of Si. The rate of trapping of hole h^+ by state S_i with the production of polaron P_i^+ is k_{1i}, while the rate of release is k_{2i}. The reaction characterizing these processes is

$$h^+ + S_i \underset{k_{2i}}{\overset{k_{1i}}{\rightleftarrows}} P_i^+. \tag{1}$$

The equations of dispersive transport of holes h^+ with the production of hole polarons P_i^+ (with their diffusion and drift in the electric field of a MOS structure taken into account) corresponding to this multiple trapping and release of holes (1) from k localized states are written as

$$\frac{\partial p}{\partial t} = D_p \frac{\partial^2 p}{\partial x^2} - \mu_p \frac{\partial (Ep)}{\partial x} - \sum_{i=0}^{k} k_{1i} C^0_{S_i} p + \sum_{i=0}^{k} k_{2i} C^+_{P_i} + G, \tag{2}$$

$$\frac{\partial C^+_{P_i}}{\partial t} = -\frac{\partial C^0_{S_i}}{\partial t} = k_{1i} C^0_{S_i} p - k_{2i} C^+_{P_i}, \quad i = 0, 1, 2, \ldots, k, \tag{3}$$

$$\frac{\partial^2 V}{\partial x^2} = -\frac{q}{\varepsilon \varepsilon_0}\left(p + \sum_{i=0}^{k} C^+_{P_i}\right), \tag{4}$$

where t is time; x is a coordinate ($x = 0$ at the gate and $x = d$ at the IPB with a silicon substrate, where d is the gate insulator thickness); p is the concentration of free (non-localized) holes; D_p and μ_p are their diffusion coefficient and mobility; $C^0_{S_i}$ and $C^+_{P_i}$ are the concentrations of ith unoccupied and filled polaron states, respectively; k is the number of localized states; V is the potential, $E = -dV/dx$ is the electric field strength, q is the electron charge; ε is the relative permittivity of silicon dioxide ($\varepsilon = 3.9$); and ε_0 is the permittivity of vacuum. Rate of production of electron–hole pairs G is specified by radiation dose rate F, coefficient of electron–hole pair production k_g, and probability $f_y(E)$ of pair separation by the electric field before their initial recombination: $G(E) = F k_g f_y(E)$, where $k_g = 1.3 \cdot 10^{-6}\,\mathrm{C \cdot cm^{-3}/rad}$. The following approximation was used for $f_y(E)$ [14]:

$$f_y(E) = \left[\frac{0.27}{(E + 0.084)} + 1\right]^{-1},$$

where E in MV/cm.

We assume that the distribution of the density of localized states over their energy has an exponential form typical of non-crystalline materials [15]:

$$C^0_{P_i}(E_{bi}) = N^0_P \exp(-E_{bi}/E_0), \tag{5}$$

where $N^0_P = C^0_S + C^+_P$ is the net concentration of unoccupied and filled polaron states, $C^0_S = \sum_{i=0}^{k} C^0_{S_i}$, $C^+_P = \sum_{i=0}^{k} C^+_{P_i}$; E_{bi} is the energy level of the ith polaron state, E_0 is the characteristic (mean) polaron energy that is related to dispersion parameter α as $\alpha = k_B T/E_0$, k_B is the Boltzmann constant, and T is temperature.

We assume that the concentrations of holes and polarons at the initial time are zero:

$$p(x, 0) = 0; \quad C^+_{P_i}(x, 0) = 0, \ i = 0, 1, 2, \ldots, k. \tag{6}$$

The boundary conditions for free holes correspond to their absorption at both $\mathrm{Si{-}SiO_2}$ and $\mathrm{SiO_2}$–gate IPBs:

$$p(0, t) = p(d, t) = 0. \tag{7}$$

Voltage V_G is applied to the gate:

$$V(0) = V_G; \quad V(d) = 0. \tag{8}$$

The threshold voltage of MOS structures is defined by the space charge in the gate insulator:

$$V_{\mathrm{th}} = -Q_{ot}/C_{ox}, \tag{9}$$

where $C_{ox} = \varepsilon\varepsilon_0/d$ is the specific capacity of the gate insulator and Q_{ot} is the effective space charge. Charges close to the silicon substrate produce a greater contribution to the threshold voltage than charges near the gate; this is taken into account in the expression for the effective space charge:

$$Q_{ot} = \frac{q}{d}\int_0^d x(p + C^+_P)dx. \tag{10}$$

We assume that all polaron states trap holes at one and the same rate: $k_{1i} = k_1 = \sigma_p v_{\mathrm{th}} D_p/D_n$, where $v_{\mathrm{th}} \cong 10^7$ cm/s is the thermal velocity of electrons and σ_p is the hole trapping cross section that depends on the electric field strength (see [16]). The following parameter values were used: $\mu_p = 2 \cdot 10^{-5}\,\mathrm{cm^2/V \cdot s}$ [7], $D_p = \mu_p k_B T$. Holes hop to a different polaron state via thermal emission at a rate of $k_{2i} = AT^2 \exp\left(-\frac{E_{bi}}{k_B T}\right)$ that depends on polaron energy E_{bi} ($A = 1.6 \cdot 10^5\,\mathrm{s^{-1}}$ is a constant). The minimum ($E_{b0} = 0.08$ eV at $T = 80$ K, $E_{b0} = 0.26$ eV at $T \geq 124$ K) and maximum ($E_{bk} = 0.55$ eV) energy levels of localized states were determined by comparing the results of calculations with experimental dependences.

3. Calculation results

Model equations (2)–(5) were solved numerically using inexplicit and explicit difference schemes with initial conditions (6), boundary conditions (7), (8), and (9) and (10) taken into account. The obtained solutions were compared to the experimental data from [5,6], where the threshold voltage of MOS transistors was measured after irradiation with electrons with an energy of 13 MeV in 4-μs-long pulses with a dose of 30 krad ($\mathrm{SiO_2}$). The irradiation temperature, external electric field strength $E_G = V_G/d$, and the thickness of gate $\mathrm{SiO_2}$ were varied.

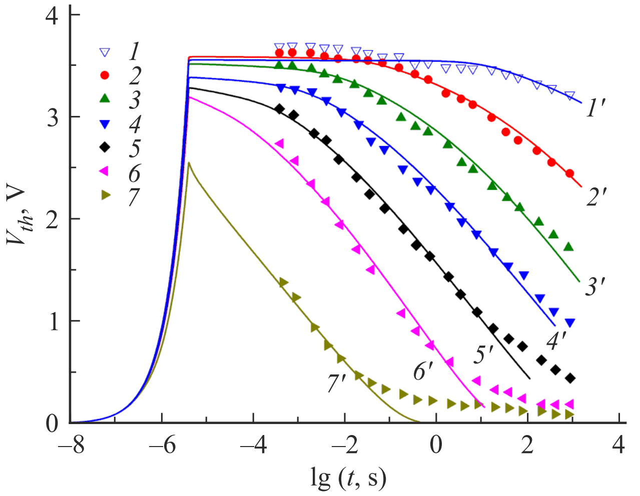

Figure 1. Influence of temperature on the kinetics of V_{th} within and after an IIR pulse, K: *1, 1'* — 124; *2, 2'* — 160; *3, 3'* — 181; *4, 4'* — 194; *5, 5'* — 217; *6, 6'* — 247; *7, 7'* — 293. Symbols *1–7* denote the experimental data from [5], while curves *1'–7'* represent the results of calculations at N_P^0, cm^{-3}: *1'* — $8 \cdot 10^{20}$, *2'* — $3.8 \cdot 10^{20}$, *3'* — $2.2 \cdot 10^{20}$, *4'* — $1.3 \cdot 10^{20}$, *5'* — $8.4 \cdot 10^{19}$, *6'* — $5.6 \cdot 10^{19}$, *7'* — $2.2 \cdot 10^{19}$. ($E_G = 1$ MV/cm, $d = 96.3$ nm, $\alpha = 0.12$). (A color version of the figure is provided in the online version of the paper).

The influence of temperature on the kinetics of shift of threshold voltage ΔV_{th} at external electric field strength $E_G = 1$ MV/cm in the process of IIR and after it is illustrated by Fig. 1. The experimental data from [5] (symbols *1–7*) and calculated curves *1'–7'* at $\alpha = 0.12$ with E_{bi} level dispersion from $E_{b0} = 0.26$ eV to $E_{bk} = 0.55$ eV are shown in this figure. Net concentration of polaron states N_P^0 was varied in calculations. It can be seen from Fig. 1 that the mean relaxation time decreases at higher temperatures due to a reduction in concentration of polaron states N_P^0.

The influence of the external electric field on the kinetics of relative shift of the threshold voltage at $T = 80$ K after IIR is illustrated by Fig. 2. The current values of shift $V_{\mathrm{th}}(t)$ are normalized to its maximum value at the initial moment of relaxation (the moment of termination of a pulse) $\Delta V_{\mathrm{th}}(0)$. Symbols *1–4* denote the experimental data from [6]. The results of calculations with E_{bi} level dispersion from $E_{b0} = 0.08$ eV to $E_{bk} = 0.55$ eV taken into account are represented by curves *1'–4'*. Characteristic polaron energy E_0 was varied in calculations. It can be seen from Fig. 2 that the mean relaxation time decreases in stronger electric fields due to a reduction in characteristic polaron energy E_0. The dependence calculated with a single level $E_{b0} = E_{bk} = 0.08$ eV is shown for comparison (curve *5'*). It can be seen that only the calculations performed with level dispersion taken into account (curves *1'–4'*) provide a satisfactory fit to the experimental data.

The influence of the gate oxide thickness on the kinetics of relative shift of the threshold voltage at $E_G = 1$ MV/cm and $T = 220$ K is illustrated by Fig. 3, which presents the experimental data from [6] (symbols *1–4*) and calculated curves *1'–4'*. Both the oxide thickness and the values of dispersion parameter α were varied in calculations. It can be seen that the mean relaxation time decreases with decreasing thickness.

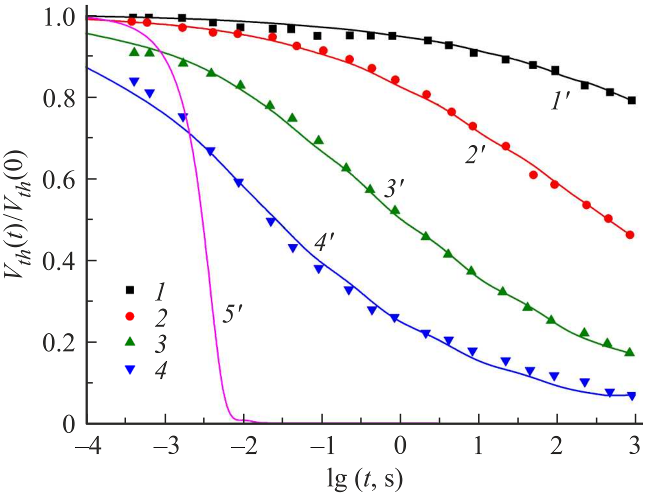

Figure 2. Influence of the external electric field strength on the $V_{\mathrm{th}}/V_{\mathrm{th}}(0)$ kinetics after an IIR pulse, MV/cm: *1, 1'* — 3; *2, 2'* — 4; *3, 3'* — 5; *4, 4'* — 6. Symbols *1–4* denote the experimental data from [6], while curves *1'–5'* represent the results of calculations at E_0, eV: *1'* — 0.047, *2'* — 0.041, *3'* — 0.034, *4'*, *5'* — 0.029. Energy levels, eV: *1'–4'* — $E_{b0} = 0.08$, $E_{bk} = 0.55$; *5'* — $E_{b0} = E_{bk} = 0.08$. ($T = 80$ K, $d = 96.3$ nm).

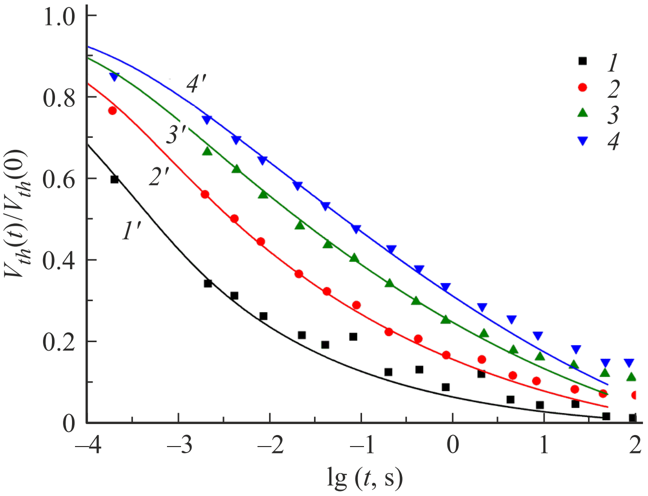

Figure 3. Influence of the gate oxide thickness on the $\Delta V_{\mathrm{th}}/V_{\mathrm{th}}(0)$ kinetics after an IIR pulse, nm: *1, 1'* — 21.8; *2, 2'* — 37.6; *3, 3'* — 56.6; *4, 4'* — 96.3. Symbols *1–4* denote the experimental data from [6], while curves *1'–4'* represent the results of calculations at α: *1'* — 0.24, *2'* — 0.17, *3'* — 0.145, *4'* — 0.145. ($E_G = 1$ MV/cm, $T = 220$ K).

4. Results and discussion

It follows from Fig. 1 that the SC relaxation time decreases at higher temperatures due to a reduction in the net concentration of polaron states. The temperature dependence of N_P^0 is presented in Fig. 4. At low temperatures, the activation energy, which is characterized by the slope of the dependence, is low: $E_a \sim 0.04$ eV at $T = 80-160$ K; as the temperature grows, E_a increases to ~ 0.13 eV at $T = 247-293$ K. This corresponds to a temperature dependence of the characteristic polaron energy specified by relation $E_0 = k_B T/\alpha$ with $\alpha = 0.12 = \text{const}$.

A similar growth of the activation energy for the threshold voltage relaxation time from $E_a = 0.06-0.1$ eV at $T < 125$ K to $E_a = 0.3-0.5$ eV at $T > 200$ K was observed in [4]. These values correspond roughly to the minimum ($E_{b0} = 0.08$ eV at $T = 80$ K and $E_{b0} = 0.26$ eV at $T \geq 124$ K) and maximum ($E_{bk} = 0.55$ eV) calculated boundaries of the polaron energy range in Figs. 1 and 2. Note that the growth of activation energy with temperature is one of the characteristic properties of polarons [4,7]. Characteristic (mean) energy E_0 may be used to estimate the mean polaron radius [17]: $r_P = \frac{q}{4\varepsilon\varepsilon_0 E_0}$. Calculations suggest that the polaron radius decreases with increasing temperature: it varies from $r_p = 200$ Å at 80 K to $r_p = 55$ Å at 293 K, but still exceeds considerably the Si–O interatomic distance (1.5–1.7 Å). Thus, contrary to the assumptions made in [7], the radius of hole polarons, which are involved with the SC accumulation and relaxation in SiO_2, is large. This result agrees with [18], where the presence of large-radius autolocalized states in amorphous SiO_2 was assumed.

It follows from Fig. 2 that the SC relaxation time decreases in stronger electric fields due to a reduction in mean polaron energy E_0. The influence of the electric field strength on E_0 is approximated by a linear dependence:

$$E_0 = 0.064 - 0.057E(\text{MV/cm}), \text{eV}.$$

This influence may be attributed to an increase in the drift velocity of holes, which eventually detach from their potential wells. Polaron states vanish in strong fields [17].

The mean relaxation time decreases with decreasing oxide thickness (see Fig. 3). This effect is associated not only with shortening of the distance to drains at both IPBs (see boundary conditions (7)), but with a change in dispersion parameter α as well. Figure 5 shows that parameter α grows from 0.145 to 0.24 as the thickness decreases. This variation of α is attributable to the presence of a stressed region (up to 30–50 nm in size), which is characterized by a rearranged structure and altered bridge angles, in thermal silicon dioxide near the IPB with silicon [19,20]. Note that the value of α is independent of temperature, but depends on the method of production of thermal silicon oxide. According to the data from [4,7], it varies from 0.14 to 0.3.

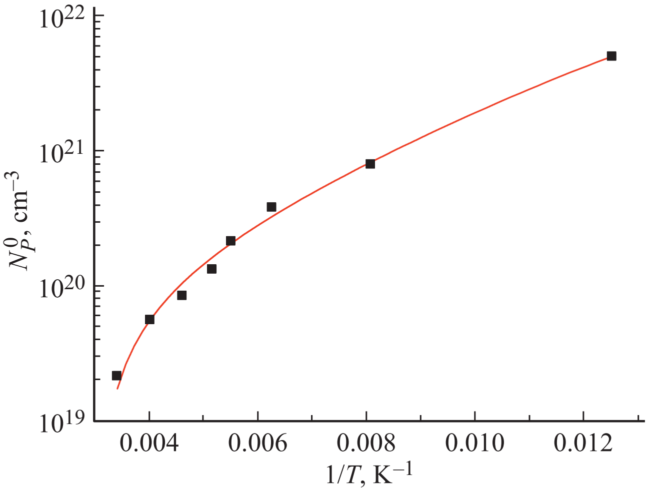

Figure 4. Temperature dependence of N_P^0. Symbols denote the data calculated for Figs. 1, 2; the curve is the result of approximation.

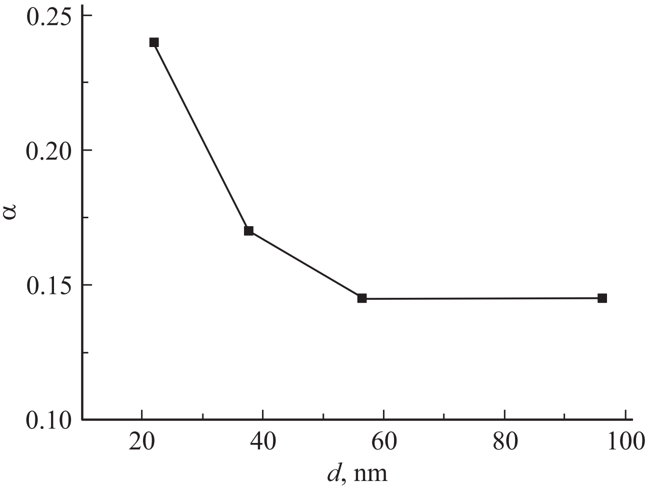

Figure 5. Dependence of dispersion parameter α on the gate oxide thickness. Symbols denote the data calculated for Fig. 3.

5. Conclusion

It was demonstrated that the multiple trapping model applied to the dispersive transport of holes provides an opportunity to characterize quantitatively the kinetics of SC relaxation in MOS structures after low-temperature ionizing irradiation. The MT theory was used to model quantitatively the temporal dependences of the threshold voltage shift on temperature, the external electric field strength, and the thickness of gate silicon oxide. It was found that the relaxation kinetics is governed by levels of localized polaron states in SiO_2 within the 0.08–0.55 eV range. The influence of a temperature rise is associated with a reduction in the concentration of polaron states. The polaron radius decreases from 200 Å at 80 K to 55 Å at 293 K, but still exceeds considerably the Si–O interatomic distance

(1.5−1.7 Å). The dependence of the threshold voltage shift on the electric field strength is induced by a reduction in the characteristic polaron energy. It was found that dispersion parameter α increases at an oxide thickness below 50 nm.

Conflict of interest

The author declares that he has no conflict of interest.

References

[1] T.R. Oldham, F.B. McLean. IEEE Trans. Nucl. Sci., **50** (3), 483 (2003).

[2] K.I. Tapero, V.N. Ulimov, A.M. Chlenov. *Radiatsionnye effekty v kremnievykh integral'nykh skhemakh kosmicheskogo primeneniya* (M., BINOM, 2012) (in Russian).

[3] O.V. Aleksandrov. Semiconductors, **55** (2), 207 (2021).

[4] F.B. McLean, N.E. Boesch, J.M. McGarrity. IEEE Trans. Nucl. Sci., **23** (6), 1506 (1976).

[5] N.E. Boesch, J.M. McGarrity, F.B. McLean. IEEE Trans. Nucl. Sci., **25** (3), 1012 (1978).

[6] N.E. Boesch, F.B. McLean, J.M. McGarrity, P.S. Winokur. IEEE Trans. Nucl. Sci., **25** (6), 1239 (1978).

[7] R.C. Hughes. Phys. Rev. B, **15** (4), 2012 (1977).

[8] H. Scher, E.W. Montrol. Phys. Rev. B, **12** (6), 2455 (1975).

[9] J. Noolandi. Phys. Rev. B, **16** (10), 4466, 4474 (1977).

[10] B. Hartenstein, A. Jakobs, K.W. Kehr. Phys. Rev. B, **54** (12), 8574 (1996).

[11] O.L. Curtis, J.R. Srour. J. Appl. Phys., **48** (9), 3819 (1977).

[12] O.V. Aleksandrov. Semiconductors, **54** (10), 1215 (2020).

[13] V.A. Gritsenko, R.M. Ivanov, Yu.N. Morokov. J. Exp. Theor. Phys., **81** (6), 1208 (1995).

[14] J.M. Benedetto, H.E. Boesch. IEEE Trans. Nucl. Sci., **33** (6), 1318 (1986).

[15] V.I. Arkhipov, A.I. Rudenko. Phil. Mag. B, **45** (2), 189, 209 (1982).

[16] R.J. Krantz, L.W. Aukerman, T.C. Zietlow. IEEE Trans. Nucl. Sci., **34** (6), 1196 (1987).

[17] N.B. Brandt, V.A. Kul'bachinskii. *Kvazichastitsy v fizike kondensirovannogo sostoyaniya* (M., Fizmatlit, 2005), p. 396 (in Russian).

[18] D.L. Griscom. J. Non-Cryst. Sol., **149** (1−2), 137 (1992).

[19] G.Ya. Krasnikov, N.A. Zaitsev. *Sistema kremnii-dioksid kremniya submikronnykh SBIS* (M., Tekhnosfera, 2003) (in Russian).

[20] O.V. Aleksandrov, A.I. Dusj. Semiconductors, **42** (11), 1370 (2008).