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Analysis of random events in physical and chemical processes flowing in materials of semiconductor products under external influences and thermal aging

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Abstract. It has been proposed to consider physical and chemical processes in materials of semiconductor products under external influences and thermal aging as flows of the random events. The mathematical analysis of random events in the physical and chemical processes has been presented. The theoretical results have been applied to the analysis of a number of processes.

Keywords: random event, random variable, distribution function of the random variable, diffusion, capture of the carrier, generation of defect, solid-phase reaction, mechanical destruction, polarization.

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1. Introduction

Exposure to electric, magnetic, electromagnetic, radiation, thermal as well as fields of mechanical stresses on materials of semiconductor products leads to a change in states of the ensembles of atoms, ions, capturing centers (traps), point and linear defects. Behavior of the mentioned ensembles in time is caused by the flow of random events in physical-chemical processes (hereinafter – random events or just events) such as motion of a particle or defect from the source to the defined boundary, changing the chemical structure of particle in chemical reactions, capture (release) of the carrier by center, generation of the defect, the decay of the interatomic bond in the mechanical destruction of solids, particle displacement during polarization of dielectrics. These events are random because at thermally activated (or thermal fluctuation) nature of the latter, they are determined by a random event such as fluctuation of a given energy of the particle of atom, ion,

molecule. On the other hand, the law of distribution of the random variable – time to each of these events – depends on whether the activation energy of events is deterministic or random value for the entire set of events. In more detail, the reasons, for which the mentioned events are random, will be discussed during the presentation.

Corresponding random events cause a change in time of the concentration inherent to reacting particles moving from the source to the defined boundary of particles or defects, filled (emptied) centers, generated defects, broken interatomic bonds, shifted particles, i.e. cause the flow of physical and chemical processes in materials of semiconductor products. Consequently, the mathematical description of random events will provide analytical expressions for the evolution kinetics of material parameters in semiconductor devices and structures under the action of corresponding fields or their termination, as well as under thermal aging.

2. Mathematical foundations of the analysis of random events in physical and chemical processes

By analogy with the reliability theory, which use the term probability of failure of the product in time t , we write the expression for the probability of the absence of any of the events for the time t [1]

$$P(t) = e^{-\int_0^t \lambda(t) dt} \quad (1)$$

where $\lambda(t)$ is the intensity of the random events in physical and chemical processes (hereinafter the intensity of events), and, by definition, at $t=0$ $\int_0^t \lambda(t) dt$ is equal to zero, while at $t \rightarrow \infty$ it also tends to infinity.

Then for the probability of the event before the time point t we have:

$$F(t) = 1 - e^{-\int_0^t \lambda(t) dt} \quad (2)$$

In other words, $F(t)$ is the function of distribution of the random variable – time to any of random events, that is the time to: changes in the chemical structure of particle, motion of particle or defect from the source to the given boundary, capture (release) of the carrier by center, generation of defect, decay of interatomic bond, particle displacement.

We interpret $\lambda(t)$ in relation to consider random events.

Similar term, but with another semantic content (failure intensity), is used in the reliability theory and is determined as follows [1]

$$\lambda(t) = \frac{f(t)}{P(t)}, \quad f(t) = \frac{dF(t)}{dt}, \quad (3)$$

where $f(t)$ is the distribution density of time to the event (the probability density of the event).

According to [1],

$$\lambda(t) = \frac{\Delta n(t)}{[n_0 - n(t)]\Delta t}, \quad (4)$$

where n_0 is the total number of events (in the physical and chemical processes, it can be arbitrarily large, but it is always limited by the number of particles, defects, centers; $\Delta n(t)/dt$ is the number of events per unit of time; $n(t)$ – number of events to the point time t .

With regard to the physical and chemical processes, the formula (4), in view of the number of events per unit volume (normalization of the number of events to the volume of material) can be written as

$$\lambda(t) = \frac{\Delta N(t)}{[N_0 - N(t)]\Delta t}. \quad (5)$$

The following defines the parameters in the formula (5) with respect to the above random events.

1. A random event is the capture (release) of the carrier by center (trap); $\lambda(t)$ is the intensity of the captures (releases) of carriers by centers; N_0 is the total concentration of the centers; $\Delta N(t)/\Delta(t)$ is the concentration of centers that have captured (released) the carriers per unit of time (the rate of captures (releases) of carriers by the centers); $N(t)$ is the concentration of filled (emptied) centers to the point time t .
2. A random event – generation of a point (linear) defect: $\lambda(t)$ is the intensity of generations of defects; N_0 is the total (equilibrium) concentration (density) of defects; $\Delta N(t)/\Delta(t)$ is the concentration (density) of defects generated per unit of time (the rate of generation of defects); $N(t)$ is the concentration (density) of the defects that have been generated to the point time t .
3. A random event – decay of the interatomic bond in the mechanical destruction of solids: $\lambda(t)$ is the intensity of decays of bonds; N_0 is the total concentration of decaying bonds; $\Delta N(t)/\Delta(t)$ is the concentration of bonds decaying per unit of time (the rate of bond decay); $N(t)$ is the concentration of bonds broken to the point time t .
4. A random event – displacement of the particle under the dielectric polarization: $\lambda(t)$ is the intensity of the displacements of particles; N_0 is the total concentration of displacing particles; $\Delta N(t)/\Delta(t)$ is the concentration of particles, displaced per unit of time (the rate of particle displacements); $N(t)$ is the concentration of particles that have been displaced to the point time t . For t so small that $N_0 \gg N(t)$, the expression (5) transforms into

$$\lambda(t) = N_0^{-1} \frac{\Delta N(t)}{\Delta t} = N_0^{-1} \nu_1(t), \quad (6)$$

where $\nu_1(t)$ is the rate of events.

Thus, at low t , the event intensity is equal to the rate of events, normalized to the total concentration of particles, defects, centers etc. In the whole range of changing time, the behavior of $\lambda(t)$ and $\nu_1(t)$ is fundamentally different.

5. An event – motion of a particle from the constant source N_0 (hereinafter – the source N_0) to a reflective boundary $x = x_0$ (hereinafter – boundary x_0) is random if it is described by the Markov (random) process. For the Markov process, the conditional probability density of transition obeys the Fokker-Planck-Kolmogorov equation (diffusion equation).

In this case, $\lambda(t)$ is the intensity of motions of particles from the source N_0 to the boundary x_0 in diffusion process; N_0 is the total concentration of diffusing particles (concentration of the constant source); $\Delta N(t)/\Delta t$ – concentration of particles moving from the source N_0 to the boundary x_0 per unit of time (the rate of motions of particles from the source N_0 to the boundary x_0); $N(t)$ – concentration of particles that have moved from the source N_0 to the boundary x_0 to the point time t .

We divide the numerator and denominator of the formula (5) by N_0 and multiply by x_0 and introduce the notations

$$x(t) = x_0 \frac{N(t)}{N_0}, \quad \Delta x(t) = x_0 \frac{\Delta N(t)}{N_0}. \quad (7)$$

The value $x(t)$ will designate the cumulated motions of particles from the source N_0 to the boundary x_0 for time t . Then the relation (5) can be written as:

$$\lambda(t) = \frac{\Delta x(t)}{[x_0 - x(t)]\Delta t}, \quad (8)$$

where $\Delta x(t)/\Delta t$ is the cumulated motion of particles from the source N_0 to the boundary x_0 per unit of time (the velocity of cumulation of motions of particles from the source N_0 to the boundary x_0).

For t so small that $x_0 \gg x(t)$, the formula (8) is transformed into

$$\lambda(t) = x_0^{-1} \frac{\Delta x(t)}{\Delta t} = x_0^{-1} v_2(t), \quad (9)$$

where $v_2(t)$ is the velocity of cumulation of events (velocity of cumulation of motions of particles from the source N_0 to the boundary x_0).

Consequently, for the analyzed diffusion process, at low t , the intensity of events is equal to the velocity of cumulation of events, normalized to the distance x_0 .

Considering the chemical transformations, we focus on solid-phase reactions (heterogeneous chemical processes) proceeding with formation and subsequent growth of new phase nuclei. Since, with respect to the solid-phase reactions, the random event is a change in the chemical structure of a particle, $\lambda(t)$ is the intensity of changes in the chemical structure of particles; N_0 – total concentration of reactive particles; $\Delta N(t)/\Delta t$ – the concentration of particles having reacted per unit of time (the rate of changes in the chemical structure of particles); $N(t)$ – concentration of particles that having reacted to the point time t .

Let's divide the numerator and denominator of the formula (5) by N_0 and multiply by V_0 (V_0 is the volume of the reaction zone). We introduce the notations

$$V(t) = V_0 \frac{N(t)}{N_0}, \quad \Delta V(t) = V_0 \frac{\Delta N(t)}{N_0}. \quad (10)$$

Then the formula (5) can be written as:

$$\lambda(t) = \frac{\Delta V(t)}{[V_0 - V(t)]\Delta t}, \quad (11)$$

where $V(t)$ is the volume (area or length) of a new phase formed to the point time t ; $\Delta V(t)/\Delta t$ is the volume of the new phase formed per unit of time (the growth velocity of a new phase).

For t so small that $V_0 \gg V(t)$, the ratio (11) has the form

$$\lambda(t) = V_0^{-1} \frac{\Delta V(t)}{\Delta t} = V_0^{-1} v_3(t), \quad (12)$$

where $v_3(t)$ is the growth velocity of a new phase.

For solid-phase reactions at low t , the intensity of events equal to the growth velocity of the new phase normalized to the volume (area, length) of the reaction zone.

Since, by the definition $F(t)$, $F(t) = n(t)/n_0$ and therefore, $F(t) = N(t)/N_0 = x(t)/x_0 = V(t)/V_0$, taking into account the expression (2) we can write

$$N(t) = N_0 \left[1 - e^{-\int_0^t \lambda(t) dt} \right], \quad (13)$$

$$x(t) = x_0 \left[1 - e^{-\int_0^t \lambda(t) dt} \right], \quad (14)$$

$$V(t) = V_0 \left[1 - e^{-\int_0^t \lambda(t) dt} \right]. \quad (15)$$

From the expressions (13)-(15), it follows that if $t \rightarrow \infty$, the values $N(t)$, $x(t)$, $V(t)$ asymptotically tend to the values N_0 , x_0 , V_0 . At low long-term physical and

chemical processes, when $\int_0^t \lambda(t) dt \ll 1$, expanding the exponential in series and limiting by the first term of the expansion, we obtain

$$N(t) = N_0 \int_0^t \lambda(t) dt, \quad (16)$$

$$x(t) = x_0 \int_0^t \lambda(t) dt, \quad (17)$$

$$V(t) = V_0 \int_0^t \lambda(t) dt. \quad (18)$$

Differentiating on t the left and right side of equations (16)-(18), we have the following relations for

$$\lambda(t) = N_0^{-1} \frac{dN(t)}{dt} = N_0^{-1} v_1(t), \quad (19)$$

$$\lambda(t) = x_0^{-1} \frac{dx(t)}{dt} = x_0^{-1} v_2(t), \quad (20)$$

$$\lambda(t) = V_0^{-1} \frac{dV(t)}{dt} = V_0^{-1} v_3(t). \quad (21)$$

These expressions are agreed with the above expressions (6), (9) and (12).

This situation can be interpreted as follows. We introduce the term – the degree of completion of a physical or chemical process α (in heterogeneous chemical processes it is the conversion degree):

$$\alpha(t) = \frac{N(t)}{N_0} = \frac{x(t)}{x_0} = \frac{V(t)}{V_0}. \quad (22)$$

The values of α range from zero to unity. Then it was at a low degree of completion of the process (conversion), when $\alpha \ll 1$, and the relations (16)-(21) are valid.

In its turn, change, which occurs in the parameters of materials and semiconductor products under the action of external fields and thermal aging, is proportional to $N(t)$, $x(t)$, and $V(t)$. And, if at the initial point time the parameter $y(t)$ have the value y_{in} , when it grows over time, taking into account (13)-(15) we will have

$$y(t) = y_{in} + y_0 \left[1 - e^{-\int_0^t \lambda(t) dt} \right], \quad (23)$$

where y_0 is the asymptotically attainable value of $y(t) - y_{in}$ when $t \rightarrow \infty$.

When reducing the parameter in time, we get

$$y(t) = y_{in} - y_0 \left[1 - e^{-\int_0^t \lambda(t) dt} \right], \quad (24)$$

where y_0 is the asymptotically attainable value of $y_{in} - y(t)$ when $t \rightarrow \infty$.

Let's consider the special case of (24), when the parameter value reduces to zero. Taking into account that the condition $y(t \rightarrow \infty) = 0$ is satisfied when $y_0 = y_{in}$, we get

$$y(t) = y_{in} e^{-\int_0^t \lambda(t) dt}. \quad (25)$$

At low long-term physical and chemical processes, such that $\int_0^t \lambda(t) dt \ll 1$ ($\alpha \ll 1$), according to (16)-(18), we obtain

$$y(t) = y_{in} + y_0 \int_0^t \lambda(t) dt, \quad (26)$$

$$y(t) = y_{in} - y_0 \int_0^t \lambda(t) dt, \quad (27)$$

$$y(t) = y_{in} \left[1 - \int_0^t \lambda(t) dt \right]. \quad (28)$$

Thus, the behavior of the parameters of materials of semiconductor devices and structures in time is determined by the form $\lambda(t)$, which is related with the type of the used distribution $F(t)$. In the probability theory, for approximation of distributions of selected data, different laws are applied, including the Weibull-Gnedenko law, normal, log-normal ones etc. For the mathematical analysis of the above random events, we use the Weibull-Gnedenko distribution [1]. Let's give a mathematical and physical basis of the applicability of this distribution, the function of which has the form:

$$F(t) = 1 - e^{-\left(\frac{t}{\tau}\right)^m}, \quad (29)$$

where m and τ are the distribution parameters (by definition $F(t)$, $m > 0$) characterizing the intensity of the events.

In accordance with (1)-(3), the expression for $\lambda(t)$ has the form:

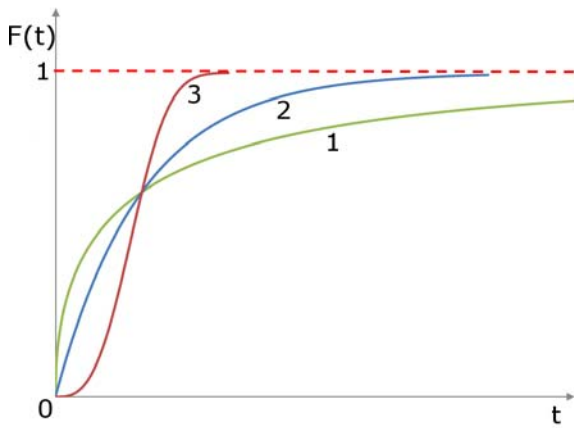
$$\lambda(t) = \frac{m}{\tau} \left(\frac{t}{\tau}\right)^{m-1}. \quad (30)$$

Hereinafter, we will refer to m a form factor of time distribution to a random event, and τ that is the scale parameter associated with the time constant of a random event. When $t = \tau$, the probability of a random event is $1 - e^{-1}$, that is about 63% of the events.

It is seen that at $m = 1$ the intensity of the events is constant, which is inversely proportional to the time of the event, and when at $m \neq 1$ it changes with time according to a power law.

The plots of the function (29) are shown in Fig. 1. It is necessary to point out three different types of behavior of the curves in the initial part of the changes in time: when $0 < m < 1$, the curve is convex, when $m > 1$, it is concave and in general it has a sigmoid (S-shaped) form, but at $m = 1$ the curve is linear.

The Weibull-Gnedenko distribution has the following important feature [2]. At $m > 1$, when $3 < m < 4$, the Weibull-Gnedenko distribution is reduced to the normal one. The Weibull-Gnedenko distribution function is symmetrical at the point $F(t) = 0.5$, when



Dependence $F(t)$ when $m < 1$ (1), $m = 1$ (2), and $m > 1$ (3).

$m = 3.26$, that is $(1 - \ln 2)^{-1}$, and the inflection point is only slowly changed with m . When $0 < m < 0.7$, the Weibull-Gnedenko distribution is a normal logarithmic one. Finally, when $m = 1$ the Weibull-Gnedenko distribution transforms into exponential one.

Let us analyze the physical and mathematical foundations of using the Weibull-Gnedenko law.

Consider the thermal activated (random) events. For these events, the time constant τ is of the form:

$$\tau = \tau_0 e^{\frac{E_a}{kT}}, \quad (31)$$

where τ_0 is the pre-exponential factor that by the order of magnitude coincides with the period of the thermal vibrations of a particle; E_a – activation energy of random event; k – Boltzmann constant; T – absolute temperature.

We assume that the activation energy for each event of the entire set of events has the same value E_a that is a determined value. In this case, the distribution function of time to the event should coincide with the distribution function of time to the energy fluctuation $E_{fl} = E_a$ of the particle (molecule, atom, ion). Really, the random variable – the time to the energy fluctuation of the particle – obeys the distribution [3]

$$F(t) = 1 - e^{-\frac{t}{\tau_{fl}}}, \quad (32)$$

where τ_{fl} is the average time between two successive fluctuations of the value $E_{fl} = E_a$ in a given particle, which is equal to [3]

$$\tau_{fl} = \tau_0 e^{\frac{E_a}{kT}}. \quad (33)$$

It is seen that the distributions (29), with taking (31) into account, and (32) coincide at $m = 1$. Thus, the law (29) with $m = 1$ is a function of the distribution before

thermal activated event, when the activation energy is a determined value.

Let us now consider the situation where the activation energy of the event is a random variable for the entire set of events.

The situation mathematically defined is reduced to the theorem by B.V. Gnedenko for limit distribution of the maximum and minimum value [1].

Consider the sequence of n distributed independent random variables t_1, t_2, \dots, t_n – times to the events with the activation energies $E_{a1}, E_{a2}, \dots, E_{an}$, where n is the number of events (the number of particles, defects, centers etc.). The distribution of each of the random variables t_1, t_2, \dots, t_n is the distribution (29) with $m = 1$, when E_a takes the values $E_{a1}, E_{a2}, \dots, E_{an}$. We form a new value ξ_n that is equal $\xi_n = \min(t_1, t_2, \dots, t_n)$, meaning by this the following: let the values t_1, t_2, \dots, t_n

took the values $t_1^*, t_2^*, \dots, t_n^*$, then for the ξ_n value we will assign a value that is equal to $\min(t_1^*, t_2^*, \dots, t_n^*)$. Let us find the distribution function, which is subject to the given value when $n \rightarrow \infty$ (in practice at sufficiently large n). According to the B.V. Gnedenko theorem [1], the limit distribution of the third type of the minimum value is the Weibull-Gnedenko distribution. Thus, and it is especially necessary to emphasize, the Weibull-Gnedenko distribution is the distribution of the random variable that is a minimum of a large number of independently operating variables.

In the theorem, the distributions of random variables are assumed to be identical. However, even if there is a difference in the distributions of the given variables, this does not preclude the use of the Weibull-Gnedenko law (29). For example, if the parameters of these distributions are different (in our case τ), then for sufficiently large n the distribution function still obeys the Weibull-Gnedenko law.

In practice, and this will be discussed below, in some cases, for explaining experimental data one use representations of the distribution by a particular law of activation energy, and thus τ . Technically, it looks like that in the exponential distribution (distribution (29) with $m = 1$), the parameter τ is also assumed to be distributed. From the viewpoint of mathematical statistics, it is fundamentally wrong, because if the random variable (in our case – time to a random event) does not obey any given distribution, it is described by another distribution, which, as it was shown, is the Weibull-Gnedenko law.

Therefore, the law (29) with $m \neq 1$ is the distribution function of time to thermal activation event, when the activation energy of the event is a random variable.

Note that in the distribution (29) with $m \neq 1$ such a value τ will figure, and hence such a value E_a which is determined from the condition that when $t = \tau$ (34).

The event probability is

$$F(t) = 1 - e^{-t}, \quad (35)$$

that is, there is observed about 63% of the events.

Replacing $\lambda(t)$ to (30) in the formulas (13)-(15) and integrating, we obtain

$$N(t) = N_0 \left[1 - e^{-\left(\frac{t}{\tau}\right)^m} \right], \quad (36)$$

$$x(t) = x_0 \left[1 - e^{-\left(\frac{t}{\tau}\right)^m} \right], \quad (37)$$

$$V(t) = V_0 \left[1 - e^{-\left(\frac{t}{\tau}\right)^m} \right], \quad (38)$$

and at t so small that $(t/\tau)^m \ll 1$, i.e., $\alpha \ll 1$ as a result of substituting (30) into (16)-(18) and subsequent integrating we will have

$$N(t) = N_0 \left(\frac{t}{\tau} \right)^m, \quad (39)$$

$$x(t) = x_0 \left(\frac{t}{\tau} \right)^m, \quad (40)$$

$$V(t) = V_0 \left(\frac{t}{\tau} \right)^m. \quad (41)$$

Substituting (30) into (23)-(25) and integrating, we obtain the following time dependences of changes in the parameters of materials of semiconductor products during physical and chemical processes

$$y(t) = y_{in} + y_0 \left[1 - e^{-\left(\frac{t}{\tau}\right)^m} \right], \quad (42)$$

$$y(t) = y_{in} - y_0 \left[1 - e^{-\left(\frac{t}{\tau}\right)^m} \right], \quad (43)$$

$$y(t) = y_{in} e^{-\left(\frac{t}{\tau}\right)^m}. \quad (44)$$

For small durations of processes $((t/\tau)^m \ll 1$, i.e. $\alpha \ll 1$), the substitution of (30) into (26)-(28), respectively, gives

$$y(t) = y_{in} + y_0 \left(\frac{t}{\tau} \right)^m, \quad (45)$$

$$y(t) = y_{in} - y_0 \left(\frac{t}{\tau} \right)^m, \quad (46)$$

$$y(t) = y_{in} \left[1 - \left(\frac{t}{\tau} \right)^m \right]. \quad (47)$$

In some cases, the time dependences (36)-(47) can be characterized by the presence of the incubation period t_0 , within which the physical and chemical processes

does not yet started. In this situation, the expressions (36)-(47) is transformed by substituting t into $t - t_0$.

Let's apply these mathematical foundations for analyzing processes occurring in the materials of semiconductor products under the action of external fields and thermal aging.

3. The model of a diffusion process

Diffusion processes occurring in semiconductor materials, dielectric films on their surface, and in the contact connections are described by the diffusion equation. The particle concentration distribution $N(t, x)$ is found by solving this equation for given initial and boundary conditions. In the case of diffusion from a constant source N_0 into the body of finite size with a reflective boundary x_0 , a function obtained on the basis of this decision $F(t) = N(t, x)/N_0$ at $x = x_0$ is the distribution function of time to motion of the particle from the source N_0 to the boundary x_0 .

It should be noted that the commonly defined boundary conditions imply a certain mathematical approximation of the real picture for process. So, the source profile of diffusing particles is not always fairly represented as a step function, as it can have a complex dependence on the coordinates. In its turn, the reflective boundary may also have a complex coordinate profile. The term "complex coordinate profile", besides, implies that it (profile) may be a random function of the coordinates.

Let in the material from the constant source N_0 with a complex coordinate profile, the particles are transported to the boundary, where they cumulate (reflective boundary), and which also has a complex coordinate profile. In this case, the distance x_0 from the source to the boundary is a random variable for the entire set of events – motions of particles from the source to the boundary.

Consider the sequence of k independent random variables t_1, t_2, \dots, t_k – times to the motions of the particles from the constant source to the reflective boundary when x_0 takes the values $x_{01}, x_{02}, \dots, x_{0k}$. The distribution of each of the random variables t_1, t_2, \dots, t_k is the function $F(t) = N(t, x)/N_0$ when $x = x_{01}, x_{02}, \dots, x_{0k}$. We form a new value ξ_k , which is equal $\xi_k = \min(t_1, t_2, \dots, t_k)$. As mentioned above, according to the B.V. Gnedenko theorem [1], the limit distribution of third type of the minimum term of the independent variables sequence is the Weibull-Gnedenko one.

Thus, the concentration of particles moving to the boundary to the point time t and the cumulated particle motions to the boundary to a given point time are subject to the relations (36), (37), (39) and (40). Accordingly, the behavior of the parameters of semiconductor structures is described by the expressions (42)-(47).

In these formulas, τ is the time constant of the motion of the particle from the constant source N_0 to the reflective boundary, and m – form factor of time distribution before motion of a particle from the constant source N_0 to the reflective boundary.

Since x_0^2/τ has a dimension of the diffusion coefficient D ,

$$\tau = \frac{x_0^2}{D}, \quad (48)$$

and, according to [4, 5] $D = D_0 \exp(-E_a/kT)$, D_0 is the pre-exponential factor.

Then the corresponding summary of formulas (36), (37), (39), (40) and (42)-(47) is as follows:

$$N(t) = N_0 \left[1 - e^{-\left(\frac{Dt}{x_0^2}\right)^m} \right], \quad (49)$$

$$x(t) = x_0 \left[1 - e^{-\left(\frac{Dt}{x_0^2}\right)^m} \right], \quad (50)$$

$$y(t) = y_{in} + y_0 \left[1 - e^{-\left(\frac{Dt}{x_0^2}\right)^m} \right], \quad (51)$$

$$y(t) = y_{in} - y_0 \left[1 - e^{-\left(\frac{Dt}{x_0^2}\right)^m} \right], \quad (52)$$

$$y(t) = y_{in} e^{-\left(\frac{Dt}{x_0^2}\right)^m} \quad (53)$$

and when $\left(\frac{Dt}{x_0^2}\right)^m \ll 1$ ($\alpha \ll 1$),

$$N(t) = N_0 \left(\frac{Dt}{x_0^2}\right)^m, \quad (54)$$

$$x(t) = x_0 \left(\frac{Dt}{x_0^2}\right)^m, \quad (55)$$

$$y(t) = y_{in} + y_0 \left(\frac{Dt}{x_0^2}\right)^m, \quad (56)$$

$$y(t) = y_{in} - y_0 \left(\frac{Dt}{x_0^2}\right)^m, \quad (57)$$

$$y(t) = y_{in} \left[1 - \left(\frac{Dt}{x_0^2}\right)^m \right]. \quad (58)$$

As x_0 is a random variable, then its value appearing in the formulas (49)-(58) is determined from (48) under

the condition that τ corresponds to that point time when according to (49)

$$\frac{N(\tau)}{N_0} = 1 - e^{-1}. \quad (59)$$

Similarly, one can use the formulas (51)-(53).

We note when the form factor m is equal to 0.5, Eq. (55) does not depend on x_0 , which is typical for the diffusion of the particles from the constant source to the semi-infinite space. Indeed, in the model of diffusion from the constant source into semi-infinite space, time motion of concentrations of particles approximately equal $N_0/2$ has the form [4, 5]:

$$x(t) = \sqrt{Dt}. \quad (60)$$

The classic example of applying these relations (49)-(58) will be given below in the section on thermally activated capture (release) of the carriers by centers.

4. Thermally activated process of filling (emptying) center (traps) with carriers

These processes occur in semiconductor structures under the influence of external fields, in particular an electric field. Electrons or ions are carriers that were captured or released by centers.

The process of filling (emptying) of the center consists of two steps – motion of the carrier to the center or from it and properly capture (release) of the carrier by the center – and is determined by the slowest step.

When the velocity of flowing process is determined by the capture (release) of the carrier by the trap, the probability of an event, that is, the time variation of the concentration of the filling (emptied) traps is described by the formulas (36) and (39), and behavior of semiconductor product parameters is subject to the relations (42)-(47). In these formulas, taking the analyzed situation into account, τ is a constant of time for capturing (releasing) the carrier by the trap (it has the form (31)), where E_a is the activation energy of capture (release) of the carrier by trap; τ_0 is the pre-exponential factor, of the order of magnitude coinciding with the period of the thermal vibrations of the carrier, and m is a form factor of time distribution to capture (release) of carrier by the trap. When $m = 1$, the intensity of captures (releases) of carriers by the traps is constant, that is, there is a thermally activated capture (release) of carriers by the centers, when the activation energy of the event is a determined value. When $m \neq 1$, the activation energy of thermally activated event is a random variable. The intensity of captures (releases) of the carriers by centers in the latter case is a power function of time.

When the slowest step in the process is motion (diffusion) of a carrier to the center or from it, the time dependence of the concentration of filled (emptied) centers are given by the expressions (49) and (54), and behavior of the semiconductor structure parameters is described by the expressions (51)-(53) and (56)-(58).

To the analyzed class of processes, we relate the Hofstein model describing the transport of ions in the layers ‘metal-SiO₂-Si’ [6]. It is based on the assumption of existence of the traps for ion charge at the interface metal-insulator. The release of ions from these traps is the slowest step in the process of charge transfer in MIS structure, determining the rate of charge cumulation in the dielectric-semiconductor interface. This model leads to the following dependence of the mirror charge in the semiconductor on time [6]:

$$Q_s = Q_0 \left(1 - e^{-t/\tau} \right), \quad (61)$$

where; $\tau = \nu^{-1} \exp(E_a/kT)$, ν is the frequency factor, E_a is the activation energy of releasing ions by the traps.

The relation (61) is fully agreed with the relation (42) at $y_{in} = 0$, $y_0 = Q_0$ and $m = 1$, that is, there is a constant intensity of releasing ions by the traps, and consequently, the activation energy of releasing ions by the traps is a determined value.

Another good example of these processes is relaxation of the conductivity ΔG of germanium due to the carrier trapping by slow centers in oxide, which, in some cases, is described by the empirical formula [7]:

$$\Delta G = \Delta G_0 e^{-(t/\tau)^{0.6}}, \quad (62)$$

and the τ temperature dependence corresponds to Eq. (48).

When analyzing the formula (62), it is indicated the important role of diffusion phenomena in the process of filling the slow centers with carriers, that is, it was assumed that the velocity of flowing process of filling the center is determined by diffusion of the carrier to it.

It was noted in [7] that the expansion (62) in series at small values of the argument gives the relaxation law in the form:

$$\Delta G = \Delta G_0 \left[1 - \left(\frac{t}{\tau} \right)^{0.6} \right], \quad (63)$$

very close to the diffusion one

$$\Delta G = \Delta G_0 \left[1 - \left(\frac{Dt}{x_0^2} \right)^{0.5} \right], \quad (64)$$

where x_0 is the thickness of oxide film; D – effective diffusion coefficient of the carriers in the oxide compound film on the surface of germanium.

Note that the expressions (62) and (63) are agreed with (53) and (58) ones when $y_{in} = \Delta G_0$ and $m = 0.6$. The agreement with the above diffusion model can be explained by the fact that the reflective boundary, to which the carriers move from the source and which is formed by the slow centers, has a complex coordinate profile due to inhomogeneous distribution of slow centers in oxide. It drew attention to the latter circumstance in the work [7].

5. Heterogeneous chemical processes (solid phase reactions)

The essence of heterogeneous chemical processes is formation of new phase nuclei and their subsequent growth [2, 8]. Nucleation is the process of forming the initial reaction interface, an important role in the course of which the lattice defects play. In its turn, the reaction interface is the area with a limited thickness equal to several lattice constants on both sides of the geometric contact surface. The reaction interface can be considered as a complex defect that partially cover reagent and is in a state of high reactivity, as preferential formation of the product occurs here.

The velocity of running any solid phase reaction is determined by either a chemical reaction, i.e. one or more steps of redistribution bonds occurring generally at the reaction interface, or transport of particles involved in the reactions to the zone of preferential reaction or from it. Also, there are possible transition areas from one to another.

Therefore, the growth of a new phase is caused by random events such as changes in the chemical structure of particles, which, according to the theory of absolute reaction rates, is thermally activated [2, 8, 9] (kinetic growth area), or the motion of particle from the source to the growing nucleus (diffusion growth area).

For small duration of growth process of a new phase ($\alpha \ll 1$) when the relation (18) is valid, that is the effects of overlapping the growing nuclei and absorbing the formed nuclei by growing ones is not affected, the expression for the amount of the reacting substance $V(t)$ has the form [2]:

$$V(t) = V_0 \int_0^t \lambda(t) dt = \int_0^t V(t, t_j) \left(\frac{dN}{dt} \right)_{t=t_j} dt_j. \quad (65)$$

And, depending on what area of the new phase growth occurs, $\lambda(t)$ is either the intensity of changes in the chemical structure of particles or the intensity of motion from the source to the growing nucleus; dN/dt is the velocity of nucleation depending on the nucleation law.

The nucleus formed to the point time t_j has the volume $V(t, t_j)$ to the point time t [2]:

$$V(t, t_j) = \sigma [r(t, t_j)]^\beta, \quad (66)$$

where β is the number of directions of an effective growth of nucleus (1, 2 or 3); σ is a factor taking into account the type and shape of the nucleus, and

$$r(t, t_j) = \int_{t_j}^t v(t) dt, \quad (67)$$

where $v(t)$ is the velocity of nucleus growth.

If the process of the nucleus growth occurs in the kinetic area (it is controlled by the process of chemical

transformation occurring at the reaction interface), $v(t)$ is a constant, and the function $r(t, t_j)$ is proportional to $t - t_j$. When the nucleus growth takes place in the diffusion area (it is controlled by the process of transferring substance), the function $r(t, t_j)$ is proportional to $[D(t - t_j)]^{0.5}$.

Substituting (67) into (66) we have [2]

$$V(t, t_j) = \sigma k_i^p (t - t_j)^p, \quad (68)$$

where k_j is the constant of the rate of the nucleus growth; p is the parameter, the values of which are presented in Table 1.

The expression for $V(t)$, and therefore, $\int_0^t \lambda(t) dt$

depends on the nucleation law.

Let's consider some of them [2, 8].

1. Instant nucleation. Nucleation occurs instantaneously at the time when appropriate experimental conditions are fulfilled

$$\begin{aligned} \text{when } t = 0, N = 0; \\ \text{when } t > 0, N = N_0, \end{aligned} \quad (69)$$

where N is the number of nuclei.

This scenario of nucleation, for example, takes place, if the lattice structural defects or impurities are nuclei of a new phase.

2. Nucleation with a constant rate

$$N = k_q t, \quad (70)$$

where k_q is the constant of the rate for the nucleation process.

3. Nucleation according to the power law

$$N = k_q^q t^q. \quad (71)$$

This nucleation law is that the stable nuclei are formed as a result of flowing several (q) stages, unlike the previous case, when the nucleus appears during one stage.

The results of integrating the expression (65) with account of (68)-(71) are shown in Table 2 [2] and

indicate the power nature of the function $\int_0^t \lambda(t) dt$. Thus,

for solid-phase reactions the time distribution to the random event obeys the Weibull-Gnedenko law.

Substituting the relations for $\int_0^t \lambda(t) dt$ into Eqs.

(15), (18), (23)-(28), for the time dependences of the cumulation of events (the volume of reacted substance) and parameters of semiconductor materials and structures, we get the expressions (38), (41), (42)-(47). In them, the form factor m of distribution of time to

random event is determined by the values p and q , and the time constant of the random event τ depends on $N_0, V_0, \sigma, A_p, A_{pq}, k_i, k_q$.

Solid-phase reactions occur in solid solutions, which, for example, are the contacts of semiconductor devices and circuits. Thus, in [10] presented are the results of research of degradation processes in rectifying contacts of the structures $(Al+Si)-n-Si$ associated with reduction in the barrier height ϕ_b . It was noted that for small duration of thermal aging, it was proportional to $t^{0.5}$, and with time increase the values of ϕ_b asymptotically approach to their minimum value.

The authors [10] attributed this behavior of barrier height to the decay of the supersaturated solid solution Si in Al and subsequent diffusion of decay products.

Assuming that the decay of the solid solution is accompanied with formation of a new phase by instantaneous nucleation and growth of one-dimensional nuclei occurring in the diffusion area, in accordance with Eq. (43), Tables 1 and 2, we have $\phi_b = \phi_{in} - \phi_0 \left\{ 1 - \exp \left[- (t/\tau)^{0.5} \right] \right\}$. For small duration of thermal aging, according to Eq. (46), we obtain $\phi_b = \phi_{in} - \phi_0 (t/\tau)^{0.5}$. This presentation is agreed with the experimental data [10].

The work [5] shows the kinetics of decay inherent to solid solutions of lithium and copper in germanium. In

the former case, the function $\int_0^t \lambda(t) dt$ is proportional to

$t^{3/2}$, and it is assumed that the new phase nuclei appear due to entering the lithium ion from the interstitial into vacancy with formation of a complex 'lithium-vacancy'. The decay rate is strongly dependent on the presence of dislocations and impurities in the crystal. For a solid

solution of copper in germanium, the function $\int_0^t \lambda(t) dt$

Table 1. The value of parameter p .

Model	Control with processes at the interface	Diffusion control
one-dimensional nuclei	1	0.5
two-dimensional nuclei	2	1
three-dimensional nuclei	3	1.5

Table 2. The expressions for the function $\int_0^t \lambda(t) dt$.

Law of nucleation	Type of the function $\int_0^t \lambda(t) dt$
instant	$V_0^{-1} N_0 \sigma k_i^p t^p$
with a constant rate	$V_0^{-1} A_p \sigma k_i^p k_q t^{p+1}$
by the power law	$V_0^{-1} A_{pq} \sigma k_i^p k_q^q t^{p+q}$

is proportional to t , wherein the rate of the recovery of copper from a supersaturated solid solution with consequent formation of local cumulations also increased in the presence of dislocations.

Since in both cases the impurities or lattice structural defects are nuclei of decay of solid solutions [5], which corresponds to the instantaneous nucleation scenario, then, in accordance with Tables 1 and 2, in the first case there was growth of three-dimensional nuclei, and in the second one – two-dimensional nuclei, which was limited by the diffusion process.

Presented in the work [11] were the results of modeling processes in the aluminum metallization of semiconductor products in the presence of electrochemical corrosion and electromigration. These processes are accompanied by the appearance and growth in the metallization of nuclei of a new phase – oxide (hydroxide) of aluminum and voids that eventually leads to breakage of metal tracks [12, 13]. The run of these processes is estimated by changing in the resistance of aluminum tracks.

Since for the failure of the semiconductor device or integrated circuit it is sufficient to break metallization only in one place and no need for its complete failure, it is possible to say that there is a situation with a low degree of conversion $\alpha \ll 1$ and, consequently, behavior of the resistance should be described by the expression (45). Indeed, as shown in [11], an increase of the resistance of metal tracks in time is described by the power functions of the form (45). Moreover, when electrochemical corrosion takes place, $m = 1.5$, which, in accordance with Tables 1 and 2 evidences the nucleation with the constant rate and diffusion control of their effective growth in one direction. When there is electromigration, $m = 2.5$, i.e. the law of nucleation is the power one with $q = 2$ and growth of one-dimensional nuclei takes place in the diffusion area.

6. Generation of point defects

Radiation and laser actions on semiconductor products give rise to point defects in materials, which are the vacancies and interstitial atoms [14-18]. The defects change the electrical properties of solids as a result of action of two mechanisms. The first one is related with formation of scattering centers for conduction electrons and is of essential importance for metals, and the second one – defects change the band structure. It is typical for semiconductors. The appearance in the band gap of the local levels (generation-recombination centers, capture centers) leads to a change in the number of charge carriers and their lifetime.

An event – generation of a defect is random, as dissipation of the energy of particles and radiation quanta in solids is a random process, caused by the non-uniform distribution of irradiation energy along the particle trajectory transferred to the solid. The result is a distribution of time before transferring to atom (ion)

located at the crystal lattice the energy, equal to the potential barrier height transition into the interstitial, i.e. the time distribution before generation of defect.

The function of time distribution to a random event determines variation in time of the concentration of generated defects, which is described by the formulas (36) and (39) and leads to a change in the parameters of materials and semiconductor devices. Summarizing the formulas that obey the kinetics of these changes has the forms (42)-(47). In the relations (36), (39), (42)-(47), τ is the time constant for generations of defects, m – form factor of distribution of time before generation of defect. If $m = 1$, the intensity of generations of defects is a constant, and when $m \neq 1$ it changes in time according to a power law.

Presented in [15] are the results of the irradiation impact on the electrical resistance of metals and alloys. The time dependences of electrical resistance growth are characterized by non-linear behavior for small durations of irradiation and limit of saturation with increasing time ($m \neq 1$ in Eqs. (42) and (45)). In some cases, there was observed a linear increase in the electrical resistance at the early stages of irradiation, indicating a constant intensity of generations of defects ($m = 1$).

The effect of various types of irradiations (γ -irradiation, electron, proton, neutron ones) on the parameters of silicon and germanium semiconductor devices is quite sufficiently systematized in [16]. Let us analyze the studies cited therein. Pre-make the following remark. The work [16] shows the dependences of the parameters of materials and devices on the integral flux of radiation Φ and the dose P that are linear functions of irradiation time.

There was a linear relationship between the change in the inverse value of the minority carrier lifetime $\Delta(1/\tau)$ in silicon and germanium for one dominant recombination center and the integral flux of irradiation (neutrons, electrons, γ -quanta) at low Φ : $\Delta(1/\tau) = K_\tau \hat{O}$, where K_τ is the coefficient of radiation change in the lifetime. This relationship is agreed with Eq. (45) in assuming constancy of the intensity of generations of defects ($m = 1$).

Behavior of the electrical resistivity of silicon and germanium in the absence of inversion of the conductivity type under condition of neutron irradiation in a certain range Φ is described by the relation $\rho = \rho_0 \exp(K_\rho \Phi)$, where ρ_0 is the ρ value before irradiation; K_ρ is the coefficient of radiation changes in the resistivity. Accordingly, for electrical conductivity we have $\sigma = \rho_0^{-1} \exp(-K_\rho \Phi)$, which follows from Eq. (44) at constancy of the intensity of generations of defects ($m = 1$).

Changing in the reciprocal static current transfer ratio in common-emitter circuit $\Delta(1/h_{21E})$ in silicon planar and germanium diffused transistors irradiated with neutrons at low Φ values when defect formation

occurs inside the semiconductor bulk is proportional to Φ , which agrees with (45) at $m = 1$.

Analysis of behavior inherent to silicon and germanium transistors of small and medium power (fused and planar) under electron, neutron, proton, and γ -quanta irradiation evidences that for large Φ deviation from linearity is observed, as indicated by Eq. (42).

In the study of the influence of surface effects on the change $1/h_{21E}$ due to the generation of surface recombination centers and space charge in the oxide film under proton, electron, and γ -radiation, the parameter characterizing the magnitude of changes in the surface recombination losses was introduced. Numerically, it is equal to the difference between $\Delta(1/h_{21E})$ and the value of change in the bulk recombination losses. For this parameter, the relationship $\Delta R_S = \Delta R_{S\text{sat}} [1 - \exp(-K_S \Phi)]$ was proposed; here $\Delta R_{S\text{sat}}$ is the ΔR_S value at saturation; K_S is the coefficient characterizing the rate of reaching saturation ΔR_S . The noted dependence is fully consistent with the dependence (42), if assuming constancy of the intensity of generations of defects ($m = 1$).

Analysis of the effect of electron, proton and neutron irradiation of powerful microwave transistors showed that a change in the critical current matching to the drop of maximum value of cutoff frequency for current transfer ratio by 3 dB is described by the expression: $I_{kp} = I_{kp0} \exp(-K_p \Phi)$ which at $K_p \Phi \ll 1$ transfers to $I_{kp} = I_{kp0} (1 - K_p \Phi)$, where I_{kp0} is the initial value of I_{kp} before irradiation; K_p is the coefficient of changes in the resistivity of the epitaxial layer of the collector. These expressions are agreed with Eqs. (44) and (47) at $m = 1$.

Impact of fast neutrons on unipolar transistors with a gate in the form of p - n transition was estimated by changing the parameters such as the cutoff voltage $U_{GS\text{cut}}$ (voltage at which the channel is overlapped), slope S , the initial drain current $I_{D\text{in}}$ (drain current at zero voltage between the gate and source). There were obtained the following relationships between these parameters and the integral flux: $U_{GS\text{cut}} = U_{GS\text{cut}0} \exp(-\bar{K}_p \Phi)$, $S = S_0 \exp(-\bar{K}_p \Phi)$, $I_{D\text{in}} = I_{D\text{in}0} \exp(-2\bar{K}_p \Phi)$, where $U_{GS\text{cut}}$, S_0 , $I_{D\text{in}0}$ are the initial values of these parameters before irradiation, respectively; \bar{K}_p is the average coefficient of radiation changes in resistivity of the channel. These dependences are a consequence of Eq. (44) at constancy of the intensity of generations of defects.

Under γ -quanta irradiation of metal-insulator-semiconductor structures, it was noted that the density of the space charge generated in the dielectric layer was nonlinearly changed and confined to the saturation limit. Also, kinetics of changes in the threshold voltage of the

radiation dose properly behaved, which is agreed with the expression (42).

Neutron and γ -quanta irradiation of silicon diodes leads to the following dependence of the reciprocal of the carrier lifetime in the base on the integral flux: $1/\tau_p = K_\tau \Phi$, where K_τ is the coefficient of radiation changes in lifetime τ_p (the expression (45) with $m = 1$).

The work [17] shows the kinetics of changes in the surface recombination velocity GaAs depending on the number of laser pulses, causing formation of defects in the material, which are responsible for the generation-recombination processes. This dependence has S-shaped configuration, that is it obeys the expression (42) with $m > 1$.

Indeed, it is rectified in the coordinates

$$\ln \ln \left\{ \left[1 - (S_r - S_{r\text{in}}) / S_{r0} \right]^{-1} \right\} \text{ and } \ln(N_p - N_{p0}),$$

where S_r is the surface recombination velocity; $S_{r\text{in}}$ – initial value of S_r ; N_p – number of laser pulses; N_{p0} – threshold number of pulses that does not change the surface recombination velocity ($N_{p0} \approx 2$). Here, tangent of the angle of slope of the line is of the order of $m \approx 2.5$. Thus, there is the intensity of generations of defects increasing with the number of pulses.

7. Formation of point defect clusters

Under the influence of radiation and in operating the micro- and nanoelectronic devices, effects of formation of point defects clusters are observed in semiconductor materials [14-16, 18]. The cluster nucleation occurs when two identical moving point defects meet together and form a fixed nucleus, on which another defects of the same type are condensed [14]. The impurity atoms and dislocations are also nuclei of clusters. In the latter case, the increased equilibrium concentration of point defects near dislocations increases the probability of local nucleation [14].

Formation of point defect clusters until the appearance of microinclusions was observed in semiconductor structures based on GaAs after their production as a result of evolution of a non-equilibrium state of defects into the equilibrium one [19].

Since formation of point defect clusters is under the scenario of solid state reactions, that is under the scheme ‘nucleation – growth’ of nuclei, for its description to attract the mathematical apparatus of heterogeneous reactions is appropriate. The diffusion rate of defects is determined by the step of clusters growth.

Accordingly, the random event is defect motion from the source of the nucleation cluster. The probability of this event determines the growth in time of cluster volume that obeys the formulas (38) and (41), where τ is the time constant of a random event, and m is the form factor of time distribution before motion of the defect

from the source to the nucleus. The data for these parameters are presented in Tables 1 and 2.

8. Generation of dislocations

Relaxation of mechanical stresses in the semiconductor products is accompanied with plastic deformation of the crystal through the mechanism of multiplication of dislocations. The mechanism of a long-term dislocation generation is, for example, the Frank-Read source [20, 21].

Practically all the crystals contain a certain amount of growth dislocations being intersected with each other form a three-dimensional grid. Frank and Reed presented the source as a moving segment of the dislocation line, which was mounted on the ends by the fixed points that are the intersection of dislocations. Also, the segregated and impurity atoms as well as fixed (sessile) dislocations can operate as the anchor points. When stresses are applied, the dislocation segment moves in the slip plane, but being fixed at the ends, it is bent, and if the stresses are above the critical (when the segment takes the form of a semicircle), the result is the formation of dislocation loop that continues to expand in its slip plane. At the same time, the initial segment restores and the whole process begins again. Slipping may occur under the influence of small stresses, at low temperatures and so fastly that diffusion in this case is inessential.

Another mechanism for generation of the dislocations was proposed by Bardeen and Hering [20]. It is based on the motion of the edge dislocation fixed at both ends, crawling over in a plane perpendicular to the Burgers vector. Generation of dislocation rings occurs similarly to the mechanism by Frank-Read and depends on the concentration of vacancies or on adding (removing) atoms from the crystal plane (planes). Such dislocation motion is solely due to diffusion motion of vacancies or atoms.

Thus, the distribution of the random variable – the time before generation of a dislocation loop (hereinafter – dislocation) – is caused by the distribution in time before motion of atom (vacancy) from the source to the dislocation segment when generating the dislocations by the diffusion mechanism or the distribution in time before the displacement of atom from the equilibrium position and bond redistribution when generating dislocation by slipping mechanism. The latter random event is complex and consists of a thermally activated event (appearance of a nucleus with double bend) and thermally activated event (expansion of double bend in both sides along the dislocation line). It should be noted that the activation energy of the appearance of a nucleus with double bend is sufficiently higher than that of bend expansion [3].

In general, semiconductor device materials are characterized by a large number of dislocation sources, for which the length of dislocation segment d is a random variable. From a mathematical viewpoint, it

means that there is a sequence of n distributed random variables t_1, t_2, \dots, t_n – the times before the generation of dislocations, when the length of dislocation segments of the total set of dislocation sources with the number n has the values d_1, d_2, \dots, d_n , respectively. We form a new value that is equal to $\min(t_1, t_2, \dots, t_n)$. Then, according to the B.V. Gnedenko theorem [1], the limit distribution of the third type of this value is the Weibull-Gnedenko one.

Similar, in mathematical terms, situation arises even if the for the total set of the dislocation sources the length of dislocation segment is a determined value, but they (dislocation segments) are under various stresses σ due to their non-uniform distribution in the semiconductor structure. Then, σ is the random variable. Accordingly, we have a sequence of n distributed independent random variables t_1, t_2, \dots, t_n – the times before generation of dislocations, when the mechanical stresses with values $\sigma_1, \sigma_2, \dots, \sigma_n$ act on the dislocation segments of the total set n of dislocation sources, respectively. Therefore, the limit distribution of the third type value equal to $\min(t_1, t_2, \dots, t_n)$ is the Weibull-Gnedenko distribution.

With the passage of time due to the blocking effect of the elastic strain fields on the sources of dislocation loops they stop functioning.

The distribution function in time before generation of dislocation determines the change in time of the dislocation density in semiconductor materials, which is described by the formulas (36), (39) and leads, in accordance with (42)-(47), to changes in the parameters of semiconductor devices. In this case, τ is the constant in time of generation of dislocation, and m is form factor of time distribution before generating dislocation. The permanent intensity of generations of dislocations takes place at $m = 1$, and when $m \neq 1$ it depends on the time.

The work [20] shows the time dependence of deformation of Ge and Si at relatively low stresses in the nonlinear (inelastic) area. The increase in deformation values over time is caused by the process of generating dislocations. These dependences are of S-shaped form and are described by Eq. (42) with $m > 1$.

We note that Eq. (43) is agreed with the results of studying slow degradation of the effective emission from LEDs based on GaP caused by the increase in time of extended non-emitting areas – defects in dark lines that are identified as dislocations. These experimental data based on the analysis of literature sources are presented in the work [22]. And as it follows from the course of the time dependence of the effective emission, m is higher than unity.

9. Mechanical destruction of solids

Destruction of solids under the influence of mechanical stresses is caused by the birth and growth of cracks in them. The essence of the destruction is sequential decay

of strained interatomic bonds caused by thermal fluctuations [3].

Changes in the concentration of molecular products of decay of interatomic bonds in time is determined by the probability of a random event – the decay of the interatomic bond – and is described by the expressions (36) and (39), where τ is the constant of time of decay of the interatomic bond, which is equal to [3]

$$\tau = \tau_0 e^{\left[\frac{(U_0 - \gamma\sigma)}{kT} \right]} \quad (72)$$

Here, τ_0 is the pre-exponential factor that by the order of magnitude coincides with the period of the thermal vibrations in the particle; U_0 – initial value of the activation energy of the interatomic bond; γ – coefficient characterizing the strength properties of solids; σ – mechanical stresses, and m – form factor of the function of time distribution before the bond decay.

When $m = 1$ (constant intensity of decays of interatomic bonds), there is thermally activated decay of interatomic bonds when the activation energy of the bond decay is a determined value. If $m \neq 1$, there observed is the thermofluctuational decay of interatomic bonds, when the activation energy of the event is a random variable.

The authors of the work [3] showed that the kinetics of cumulation of molecular interatomic bond decay products (stable end groups and stable radicals) in polymers under mechanical stresses can be approximated using the expressions (36), (39) at $m = 1$ and more complex dependences ($m \neq 1$). In this case, in [3] the attention was paid to the fact that the situation with $m = 1$ (constant intensity of decays of interatomic bonds) can be observed only when all the particles and events occurring with them are the same, that is, all acts occur with the same activation energy (activation energy of interatomic bond decay – determined value). If the particles of different types in the system are mixed, their decay occurs with different activation energies (activation energy of interatomic bond decay – a random variable), then $m \neq 1$.

The latter situation, as pointed in [3], is caused by the fact that a random variable is the stress in the interatomic bond. Indeed, according to Eq. (72), $E_a = U_0 - \gamma\sigma$, and therefore, if σ is the random variable, then E_a is also a random variable.

In this case, the particles are non-identical with respect to their ability to decay: in one particles – the activation energy is lower (where tensile forces are greater), in others – higher. In this sense, the loaded material is a system of a mixture of “unequal” particles, i.e. particles with different activation energies of their decay.

In crystalline solids, thermofluctuational decay of strained interatomic bonds is most adequately described with the assistance of dislocation models [3]. When cumulating the random events – generation of dislocations under the influence of mechanical stresses –

their clusters arise and appearance of microcracks becomes possible. So, if the number of similar dislocations is stopped by obstacle, the large over stresses near the leading dislocation are the cause of the random event – thermal activated decay of the interatomic bond, and hence, formation of the microcrack. In the basis of microcrack formation, there may be a thermally activation event – appearance of the double bend nucleus in the dislocation with following merger of this bend and then of whole dislocation through the thermally activated event – expansion of the double bend in both sides along the dislocation line with neighboring dislocation. After microcrack formation, the cumulated dislocations due to the flow of the random events – thermofluctuation pushings – begin gradually to go into it. Since when growing the cracks, the blocked dislocation sources are released and begin to operate, the process of crack growth is accompanied by plastic deformation.

The crack development itself is jump-like. Each jump in the slip plane, which feed the crack, redistributes stresses, which followed by a flow of random events – thermofluctuation pushings of dislocations into the cracks. When the crack reaches the neighboring slip plane, its growth slows down, and then after the jump-like transition of the crack peak through the slip plane into the stretched area of the crystal, the growth of the crack again accelerates, and the development of the process is again repeated.

Since in the described scenario of strained interatomic bonds decay in crystalline solids, the random event – the interatomic bond decay – is caused by the random event – generation of dislocations, the increase of the concentration of broken bonds in time is again described by the expressions (36) and (39).

10. Polarization of dielectrics

Under polarization, we understood displacement of charged particles under the influence of an external electric field, leading to the appearance of the electric moment. In polarization, electrons, ions, dipoles can participate. The mechanism of setting the polarization can be deformation, relaxation (through thermal fluctuations), migration one [23, 24].

Hereinafter, we will consider the relaxation polarization. The change in time of the concentration of displaced particles (relaxators) under the influence of an electric field is determined by the probability of thermally activated event – particle displacement – and is described by the expressions (36) and (39), where τ is the time constant of displacement of particle (relaxator), and m is the form factor of the function of time distribution before displacement of the particle (relaxator).

When $m = 1$, the intensity of the displacements of particles is constant, that is, the activation energy of the random event – thermally activated particle

displacement – is a determined value. When $m \neq 1$, the activation energy of thermally activated event is a random variable.

Consequently, the process of setting polarization in dielectrics is described by the expression (42), here $y(t) = P(t)$, $y_{in} = 0$, $y_0 = P_0$, where $P(t)$ is polarizability; P_0 is steady value of polarizability, that is,

$$P(t) = P_0 \left[1 - e^{-\left(\frac{t}{\tau}\right)^m} \right]. \quad (73)$$

Formula (73) with $m = 1$ (constant intensity of the displacements of particles) transforms into the well-known relation for setting relaxation polarization under electric field [23, 24]

$$P(t) = P_0 \left(1 - e^{-t/\tau} \right), \quad (74)$$

and, when switching off the electric field in dielectrics with steady polarizability, the time kinetics, according to (44) with $m = 1$, has the form [24]

$$P(t) = P_0 e^{-t/\tau}, \quad (75)$$

where $\tau = \nu^{-1} \exp U/kT$; U is the height of the potential barrier that is overcome by the particle during relaxation (activation energy of the particle displacement); ν is the frequency factor that by the order of magnitude coincides with the frequency of the particle thermal vibrations.

The analysis of different material dielectric spectra based on the Cole-Cole diagrams shows their deviations from the semicircle (blurring of the spectrum dispersion) [24], that is, from the regularities predicted by the formulas (74) and (75), which led to the need to make assumptions about the distribution of relaxators [24]. So, in [24] a normal (Gaussian) distribution for the heights of the potential barrier that is overcome by particles during relaxation was used.

As already mentioned, technically it looks like that in the exponential distribution (the distribution (29) with $m = 1$), which is the basis of Eqs. (74) and (75), the parameter τ is also assumed to be distributed. From the viewpoint of mathematical statistics, it is fundamentally wrong, as if the random variable (in our case – time to the particle displacement) does not obey any one distribution, it is approximated by the other distribution. In this situation, it is the Weibull-Gnedenko distribution and, accordingly, the expression for finding $P(t)$ has the form (73).

It should be noted that a similar pattern was also observed when analyzing thermally stimulated current relaxation, whereas for explanation of the obtained results, attracted was the presentation about the distribution of electrically active defects by the activation energy and frequency factor [25], which is characterized by a marked disadvantage.

11. Conclusions

Thus, the physical and chemical processes occurring in the materials of semiconductor products under the influence of external fields and thermal aging are caused by corresponding random (thermofluctuation) events. Time regularities of processes are determined by the distribution function of the random variable – the time to a random event. It is shown that as the given random variable is the minimum of the large number of independent operating quantities, then such distribution is the Weibull-Gnedenko one. For thermally activated events, when the activation energy of the event is the determined value, the form factor of Weibull-Gnedenko distribution is equal to unity, and it turns into an exponential distribution. In a general case, if the activation energy of the event is random variable, the form factor is not equal to unity. This presentation allowed from uniform (probability) positions to give a mathematical description of the time evolution of a number of physical and chemical processes. Proposed is the mathematical model of the flowing diffusion when the profiles of source of diffusing particles and boundary, to which they move, are not a step function, but have a complex dependence on coordinates, i.e. are a random function of the coordinates. Presented were the analytical expressions for evolution of the parameters of materials and semiconductor products in the thermally activated process of filling (emptying) of traps (center) with carriers, mechanical destruction of solids, relaxation polarization of dielectrics in the situations where the activation energy of a random event is a determined and random variable. Described were of the development in time of the processes of generation of linear defects – dislocations provided that the length of dislocation segment or the value of acting on it mechanical stress is a random variable. With the proposed position, the analyzing were flowing heterogeneous chemical processes (solid-state reactions), the essence of which is formation and growth of nuclei from a new phase. The resulting expressions for the time kinetics coincide with those obtained in other ways, which take into account the effects of overlapping inherent to growing nuclei and absorption of the creating nuclei by growing ones. The work presents the analytical relations for the time dependences for behavior of the material and semiconductor device parameters, when point defects are generated under the influence of irradiation. Quite extensive analysis of various literature sources has shown agreement of the obtained theoretical results with the experimental data.

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