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SEMICONDUCTOR STRUCTURES, LOW-DIMENSIONAL SYSTEMS, AND QUANTUM PHENOMENA

Domain-Size Evolution upon Switching of the States of a One-Dimensional System with Defects

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Abstract—The decay kinetics of metastable states in highly perfect materials is well described by Kolmogorov–Johnson–Mehl statistical theory. We generalize this theory to a one-dimensional system with regard to the effect of chaotically distributed defects that hinder new phase propagation. We calculate a phase transformation pattern that is randomly inhomogeneous in space and time depending on the density of defects and delay times caused by them. The theory is applicable to the extended contacts of large-scale integrated circuits, magnetic nanowires, quasi-one-dimensional semiconductors encapsulated in carbon nanotubes, biological macromolecules, and many other systems.

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1. INTRODUCTION

There exist various linear systems of different nature whose states change according to the formation of preferred-state nuclei (domains), their growth and merging, which occur randomly in space and time. Among such transformations are the switching of magnetization in nanowires [1], dislocation drift from the crystal-relief valley [2], DNA molecule replication [3], polymer relaxation [4], and many other physical, chemical, and biological examples. The intensive development of the technology of using carbon nanotube for the growth of quasi-one-dimensional crystals yielded an increased number of objects for studying the kinetics of phase transformations in such systems [5–7]. State switching kinetics plays an important role in linear systems of information recording and readout [8].

Domain walls are often interpreted as soliton-like formations (kinks) and domain merging, as the annihilation of kink solitons bordering the domains. A nontrivial point/aspect in the description of this problem is the necessity of taking into account the coalescence of domains of different sizes created at different chaotic instants of time at random spatial points. Despite the fact that Kolmogorov formulated the approach to solving this problem and obtained a result for rather perfect systems in as early as 1937 [9], erroneous interpretations continue to be met in publications (see discussion in [10, 11]). This evokes special interest in describing in more detail the evolution of systems in the transition state.

The transformation kinetics described as a temporal variation in a fraction of a transformed substance were calculated in study [9] (see also [12]). Various applications of this theory have been described in a vast and increasing number of studies (see reviews [10, 13] which are still far from being exhaustive). Further, the spatial structure of perfect systems during switching was studied, i.e., the statistical size distribution of domains [14–17]. These studies laid the foundation for a new field of science called geometric probabilities [18].

In real systems, the effect of defects on the transformation kinetics is important. Defects can serve as both domain nucleation centers and obstacles to domain propagation. The effect of defects on the temporal variation in a transformed-substance fraction was investigated in [19–22]. In this study, we investigate the effect of defects on the space–time pattern of a transformation in one-dimensional systems. We calculate the evolution of the size distribution of domains of the initial phase and the kinetics of the change in the average sizes of the new phase. The development of electron microscopy methods for in situ visualization of nanosystem dynamics [7] makes such a calculation topical.

2. MODEL DESCRIPTION

In the initial Kolmogorov–Johnson–Mehl model, a situation is considered where the driving force of the process is sufficiently large, so stable domains of a new phase are nucleated in a small, so-called critical, volume of the initial medium independent of one another. This stage of the process is described by specifying the frequency J of domain creation in unit time per unit system length. Further growth of the nuclei can be described in terms of domain-wall motion with a certain drift velocity v. Thus, to make the model applicable, the average domain-wall path until mutual annihilation should exceed by far the critical nuclei size.

Two cases most frequently considered in the theory are the following [10]. The first case is time homogeneous nucleation with a constant rate in unit time per

unit length, $J = \text{const}$. The second case corresponds to the situation where nuclei simultaneously appear only at the initial instant of transformation, $J = I\delta(t)$ [23]. This situation is implemented, in particular, when nucleation occurs at active centers (impurities etc.). In [24, 25], this process was studied as applied to the formation of pairs of domain walls (kink solitons). To cover both of these cases, as well as other possible cases, we will consider $J(t)$ as a general function [9]. A natural constraint is the finiteness of the number of nuclei forming in finite time, which is expressed by the integral convergence condition

$$I(t) = \int_0^t dt' J(t').$$

The velocity of domain-wall motion v is assumed to be constant.

In the absence of defects, nuclei created in the time dt' per unit system length in the amount $J(t')dt'$ will expand by the instant of time t to the size $2v(t - t')$, because in the initial stage, before the domain collisions start, a new phase fraction grows as

$$2\int_0^t dt' J(t')\, v(t - t').$$

According to the general result of Kolmogorov [9], accounting for domain collisions and coalescence leads to the fact that at a later stage the new phase fraction grows as $1 - Q_0^2(t)$, where $Q_0(t)$ is

$$Q_0(t) = \exp\left[-\int_0^t dt' J(t')\, v(t - t')\right] = \exp[-vtI(t) + vI_1(t)]. \quad (1)$$

Here,

$$I(t) = \int_0^t J(t')dt', \quad I_1(t) = \int_0^t J(t')t'dt'.$$

The average transition time is

$$t_{av0} = \int_0^\infty dt Q_0^2(t) = \int_0^\infty dt \exp[-2vtI(t) + 2vI_1(t)]. \quad (2)$$

If $J(t) = I\delta(t)$, then $Q_0(t) = \exp\{-vIt\}$ and $t_{av} = 1/(2vI)$. The other type of the dependence is illustrated by $J(t) = J_\mu t^\mu$ ($\mu > -1$). In this case, we may take $t_{0\mu} = 1/(vJ_\mu)^{1/(\mu+2)}$ as the time scale. We have

$$Q_0(t) = \exp[-vtI(t) + vI_1(t)] = \exp\left[-\frac{1}{(\mu+1)(\mu+2)}\left(\frac{t}{t_{0\mu}}\right)^{\mu+2}\right], \quad (3)$$

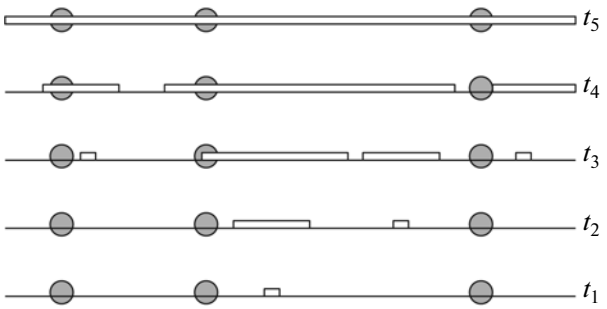

Fig. 1. Schematic of system state switching by the formation of new phase nuclei (domains), their broadening, and merging in successive instants of time t_1, ... Circles show the defects hindering domain-wall motion.

$$t_{av} = \int_0^\infty dt \exp\left[-\frac{2}{(\mu+1)(\mu+2)}\left(\frac{t}{t_{0\mu}}\right)^{\mu+2}\right] = t_{0\mu}\left[\frac{\mu+1}{2(\mu+2)^{\mu+1}}\right]^{1/(\mu+2)}\Gamma\left(\frac{1}{\mu+2}\right). \quad (4)$$

Here, $\Gamma(x)$ is the gamma function (see, for example, [26]).

Below, we use also the probability $q(t, l)$ of the fact that the considered point is not trapped by the new phase due to the formation of a nucleus only adjacent to either side of a segment with the length $l < vt$, which is smaller than the path length vt. Within the Kolmogorov approach, this value is calculated as

$$q(l, t) = \exp\left[-\int_0^{t_l} dt' J(t')l - \int_{t_l}^t dt' J(t')\, v(t - t')\right] = \exp[vt_l I(t_l) - vtI(t) - vI_1(t_l) + vI_1(t)], \quad t_l = t - l/v. \quad (5)$$

The fraction of the initial phase $Q_0^2(t)$ remaining to the time t is also the probability of the fact that the given point belongs to an initial phase spacing of any length. In the studies [14–17], a more detailed characteristic was calculated: the size distribution of the initial phase spacings for ideal linear systems. In the subsequent sections, we generalize this calculation to systems with defects hindering domain-wall motion. Simultaneously, we simplify the derivation of the results for ideal systems.

3. KINETICS OF THE INITIAL PHASE DECREASE IN THE PRESENCE OF DEFECTS HINDERING DOMAIN-WALL MOTION

Figure 1 schematically represents the different stages of the transformation process: the formation of the new phase nuclei, their broadening accompanied with overcoming the obstacles created by defects, and

coalescence. We assume that defects are randomly distributed in space with an average density of n and the delay created by them has a random duration with an average value of τ. In study [19], using another method, a situation was considered where the delay-time spectrum slowly decreases at long times, which leads to anomalous domain-wall motion. The case of a fixed delay time was considered in the self-consistent time approximation in [20] and, in more detail, in [21]. In this study, we derive a general equation for the arbitrary function of the delay-time distribution.

We calculate the one-sided probability $Q(t)$ of some point not being trapped by the new phase (for certainty, on the right, if the system is conventionally horizontal) at the time t. We denote the additional to $Q(t)$ probability of the considered point being trapped due to nuclei formation on either side as $P_1(t) = 1 - Q(t)$. Let the first defect be located to the right of the considered point at a distance of l. Then, at $l > vt$, the defect does not affect the point and the probability of not being trapped is the same as in the defect-free case, i.e., $Q_0(t)$. The probability of a lack of defects in the spacing vt is $\exp(-nvt)$.

If the first defect is closer than vt, we should take into account the possibility of the fact that the wall which approached the defect in the instant of time t' may be held at it for a time longer than $t - l/v - t'$ and, consequently, may not have time to pass the origin of coordinates by the time t. We denote the probability of being delayed by a defect for longer than t as $f(t)$ and calculate the probability of the wall not being to the left of the defect by the time $t_l = t - l/v$. We denote this probability as $Q_-(t_l)$. It amounts to the sum of the probability of the wall not approaching the defect by the time t_l, i.e., $Q(t_l)$, and the probability of the fact that, having approached the defect in the time dt', the wall does not overcome it for the time $t_l - t'$ for all t' within $(0, t_l)$, i.e., $dP_1(t')$:

$$\begin{aligned} Q_-(t_l) &= Q(t_l) + \int_0^{P_1(t_l)} f(t_l - t')(dP_1(t') \\ &= Q(t_l) - \int_1^{Q(t_l)} f(t_l - t')dQ(t') \\ &= f(t_l) + \int_0^{t_l} \frac{df(t_l - t')}{dt'} Q(t')dt'. \end{aligned} \tag{6}$$

Taking into account the entire spectrum of possible locations of the first obstacle, we obtain the equation

$$Q(t) = \exp(-vtn)Q_0(t) + n\int_0^{vt} dl. \tag{7}$$

Now, we pass from integration over l to integration over t_l:

$$Q(t) = \exp[-vtn + vI_1(t) - vtI(t)]$$
$$\times \left\{1 + nv\int_0^t dt_l \exp[nvt_l + vt_lI(t_l) - vI_1(t_l)]Q_-(t_l)\right\}.$$

Replacing the exponent on the left-hand side of the equality and differentiating both sides, we arrive at

$$\frac{dQ(t)}{dt} + [nv + vI(t)]Q(t) = nvQ_-(t). \tag{8}$$

Substitution of $Q_-(t)$ from (6) in (8) yields a closed equation relative to $Q(t)$ at an arbitrary function of the delay-time distribution $f(t)$.

Below, we consider the random time-homogeneous probability of overcoming obstacles with an average frequency of $1/\tau$. In such a situation corresponding, for example, to the thermoactivated kinetics of overcoming similar obstacles, the probability of the delay time exceeding t is $f(t) = \exp(-t/\tau)$. Then, Eq. (6) acquires the form

$$\frac{dQ_-(t)}{dt} + \frac{1}{\tau}Q_-(t) = \frac{1}{\tau}Q(t). \tag{9}$$

Excluding $Q_-(t)$ from system (8)–(9), we obtain the closed differential equation for $Q(t)$:

$$\frac{d^2Q(t)}{dt^2} + [nv + 1/\tau + vI(t)]\frac{dQ(t)}{dt} + [Jv + vI(t)/\tau]Q(t) = 0. \tag{10}$$

Note that, at $n = 0$ or at finite n but $\tau \longrightarrow 0$, which corresponds to the transition to the ideal system, the function $Q_0(t)$ satisfies Eq. (10). On the other hand, at $n \longrightarrow \infty$, $\tau \longrightarrow 0$, and finite $n\tau$, retaining only the principal terms in (10), we obtain the equation

$$(nv + 1/\tau)\frac{dQ(t)}{dt} + (vI(t)/\tau)Q(t) = 0,$$

whose solution is

$$Q(t) \approx \exp\left\{-\frac{v}{1 + nv\tau}[tI(t) - I_1(t)]\right\}. \tag{11}$$

This result differs from (1) merely by the renormalization of the velocity of domain-wall motion, which is only natural, since, in the limiting case, the wall path before annihilation is large as compared with the average distance between obstacles and the self-average of the velocity. In the general case, such self-averaging does not occur, so fluctuations in the random distribution of defects are significant.

Let us consider some particular situations that supplement the case of the average creation frequency $J =$ const considered in detail in [21].

(I). $J(t) = I\delta(t)$. Equation (10) becomes an equation with constant coefficients and is easily solved. The δ-function contribution in Eq. (10) is transformed to the initial condition $\left.\frac{dQ(t)}{dt}\right|_{t=0} = -\nu I$. The general solution is written in the form of a linear combination of the exponents:

$$Q(t) = C_1\exp(k_1 t) + C_2\exp(k_2 t), \tag{12}$$

$$k_{1,2} = -\frac{1}{2}(\nu n + \nu I + I/\tau) \pm \left[\frac{1}{4}(\nu n + \nu I + 1/\tau)^2 - \nu I/\tau\right]^{1/2}. \tag{13}$$

It follows from the initial conditions that

$$C_1 + C_2 = 1, \quad k_1 C_1 + k_2 C_2 = -\nu I, \tag{14}$$

Then,

$$C_1 = \frac{k_2 + \nu I}{k_2 - k_1}, \quad C_2 = -\frac{k_1 + \nu I}{k_2 - k_1}. \tag{15}$$

The average transformation time is

$$t_{av} = \int_0^\infty dt Q^2(t) = -C_1^2/(2k_1) - C_2^2/(2k_2) - 3C_1C_2/(k_1 + k_2). \tag{16}$$

(II). $J(t) = J_\mu t^\mu$ ($\mu = 0$ corresponds to the case of the constant average creation frequency $J = \text{const}$ considered in [21]).

As the time scale, we take $t_{0\mu} = 1/(\nu J_\mu)^{1/(\mu+2)}$; as the length scale, $l_{0\mu} = [\nu^{\mu+1}/J_\mu]^{1/(\mu+2)}$. We introduce the dimensionless time $t' = t/t_{0\mu}$ and the dimensionless parameters $n \longrightarrow n' = n/n_{0\mu}$, $n_{0\mu} = 1/l_{0\mu}$, and $\tau \longrightarrow \tau/t_{0\mu}$. Equation (10) acquires the form

$$\frac{d^2Q(t')}{dt'^2} + \left(n' + 1/\tau' + \frac{t'^{\mu+1}}{\mu+1}\right)\frac{dQ(t')}{dt'} + \left[t'^\mu + \frac{t'^{\mu+1}}{(\mu+1)\tau'}\right]Q = 0. \tag{17}$$

The numerical solution of Eq. (17) at $\mu = -1/2$ is illustrated in Fig. 2. It can be seen that an increase in the defect density slows the transformation process as compared with the case of a pure material. An increase in the average delay time also slows the transformation kinetics, but with saturation of the effect at $\tau \longrightarrow \infty$.

Evidently, this slowdown also occurs in the general case at any domain creation frequency $J(t)$ and leads to a decrease in the time derivatives of $Q(t)$. For this reason, at large n the contribution of the second derivative $\frac{d^2Q(t)}{dt^2}$ to Eq. (10) is small and can be omitted. The simplified equation is easily solved; the approximate solution is written as

$$Q(t) \approx \exp\left[-\int_0^t dt' \frac{J(t')\nu + \nu I(t')/\tau}{n\nu + 1/\tau + \nu I(t')}\right] = \frac{1}{1 + \nu I(t)/(n\nu + 1/\tau)} \times \exp\left[-\frac{t}{\tau} + \frac{1}{\tau}\int_0^t \frac{n\nu + 1/\tau}{n\nu + 1/\tau + \nu I(t')} dt'\right]. \tag{18}$$

At relatively short times when the density of obstacles is large as compared with the density of already formed nuclei $I(t)$, expression (18) transforms into expression (11) which differs from $Q_0(t)$ merely by renormalization of the average domain-wall velocity. At long times and, correspondingly, high density of formed nuclei, the form of the solution principally

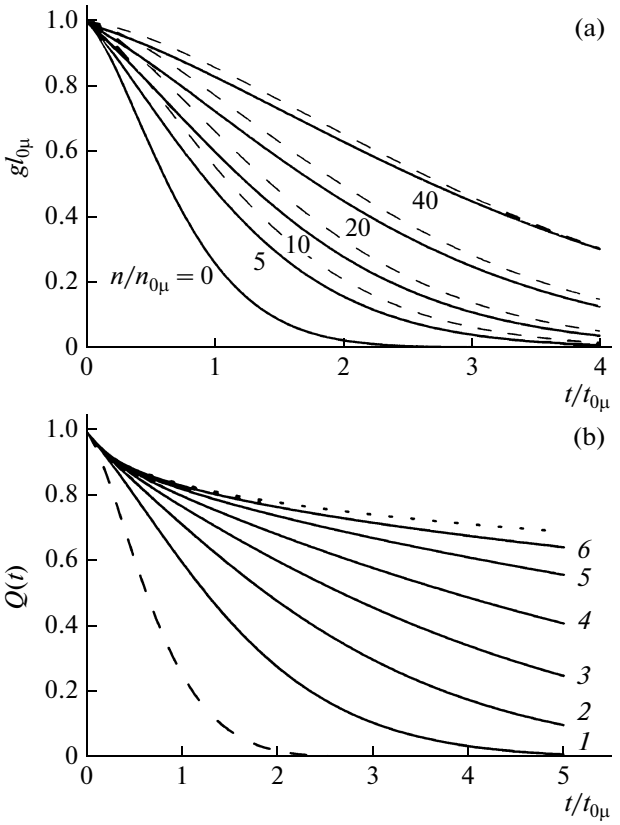

Fig. 2. Characteristics of a decrease in the initial phase fraction $Q(t)$ at $\mu = -1/2$ for (a) different dimensionless defect densities $n/n_{0\mu}$ given near the curves (dashed lines show approximate solutions according to Eq. (21) $r = 0.2t_0$) and (b) average delay times $\tau/t_{0\mu}$ of (*1*) 0.2, (*2*) 0.5, (*3*) 1, (*4*) 2, (*5*) 5, and (*6*) 15. $n/n_{0\mu} = 10$. The dashed line corresponds to a lack of defects and the dotted line, to the limit $\tau \longrightarrow \infty$.

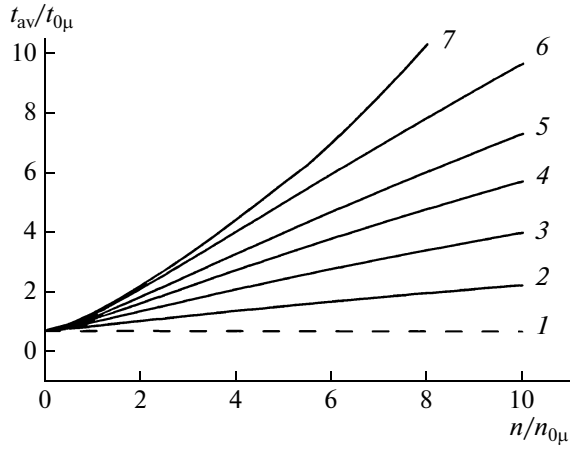

Fig. 3. Average transformation time vs defect density at $\mu = -1/4$ for delay times $\tau/t_{0\mu}$ of (*1*) 0, (*2*) 1, (*3*) 4, (*4*) 10, (*5*) 20, (*6*) 50, and (*7*) ∞.

changes, which is illustrated below by specific examples.

In the specific case $J(t) = J_\mu t^\mu$, using hereinafter the dimensionless time $t' = t/t_{0\mu}$, we have

$$Q(t) \approx \frac{1}{1 + t'^{\mu+1}/[(\mu+1)(n' + 1/\tau')]} \times \exp\left[-\frac{t'}{\tau'} + \frac{1}{\tau'} f_1(t')\right]. \quad (19)$$

$$f_1(t) = \int_0^t \frac{n' + 1/\tau'}{n' + 1/\tau + t'^{\mu+1}/(\mu+1)} dt' = \frac{t'}{\mu+1} \Phi\left(-\frac{t'^{\mu+1}}{(\mu+1)(n' + 1/\tau')}, 1, \frac{1}{\mu+1}\right).$$

Here,

$$\Phi(z, 1, v) = \sum_{k=0}^{\infty} \frac{z^k}{n+k}$$

is the degenerate hypergeometric function (see 1.2.4.2. in [26]).

At $\mu = 0$,

$$f_1(t) = -(n' + 1/\tau')\left[-\frac{t'}{n' + 1/\tau'}\right]\Phi\left(-\frac{t'}{n' + 1/\tau'}, 1, 1\right) = (n' + 1/\tau')\ln\left(1 + \frac{t'}{n' + 1/\tau'}\right).$$

As a result, according to [21], we obtain

$$Q(t) = \exp(-t/\tau)\left[1 + \frac{t(vJ_0)^{1/2}}{n' + 1/\tau'}\right]^{(n' + 1/\tau')/\tau' - 1}. \quad (20)$$

At $\mu = -1/2$,

$$f_1(t) = \int_0^{t/t_{0\mu}} \frac{n' + 1/\tau'}{n' + 1/\tau' + 2t'^{1/2}} dt' = (n' + 1/\tau') \times \left[(t/t_{0\mu})^{1/2} - \frac{n' + 1/\tau'}{2}\ln\left(1 + \frac{2(t/t_{0\mu})^{1/2}}{n' + 1/\tau'}\right)\right]. \quad (21)$$

$$Q(t) \approx \exp[-t/\tau + (n' + 1/\tau')(t/t_{0\mu})^{1/2}/\tau'] \times \left(1 + \frac{2\sqrt{t/t_{0\mu}}}{n' + 1/\tau'}\right)^{-(n' + 1/\tau')^2/2\tau'}.$$

Having calculated the function $Q(t)$, we obtain the time dependence of the new phase fraction $1 - Q^2(t)$, which allows us to find the average transformation time

$$t_{av} = \int_0^\infty dt Q^2(t).$$

Figure 3 shows the behavior of t_{av} as a function of the problem parameters. As the average delay time τ increases, the transformation time increases, approaching saturation. The kinetics becomes especially sensitive to fluctuations in the spatial distribution of defects and, depending on the time behavior of the domain-creation frequency $J(t)$, different types of system evolution become possible.

4. TRANSFORMATION KINETICS AT ULTIMATE STRONG HINDRANCES

For long delay times $\tau \longrightarrow \infty$, the probability of preservation of the initial phase can be affected only by the domains created before the first obstacle. The contribution of the spacing with the length $l > vt$ to $Q(t)$ is $\exp(-nvt)Q_0(t)$; spacings with $l < vt$ make the contribution

$$n\int_0^{vt} dl \exp(-nl) q(l, t),$$

which corresponds to substitution of the probability of is the obstacle not being overcome $Q_-(t_l) = 1$ in Eq. (7). Consequently, for $Q(t)$ within this limit we obtain

$$Q(t) = \exp(-nvt)Q_0(t) + n\int_0^{vt} dl \exp(-nl) q(l, t). \quad (22)$$

At large n, the main contribution to integral (22) is made, as can be easily seen, by relatively small values of l, so we can expand the exponent in $q(l, t)$ taking only the linear terms. We obtain

$$Q(t) \approx \exp(-nvt)Q_0(t) + \frac{n}{n + I(t)}\{1 - \exp[-(n + I(t))vt]\},$$

which transforms, after a relatively short initial stage $t \approx 1/n\nu$, to

$$Q(t) \approx \frac{n}{n + I(t)}. \quad (23)$$

This formula is interpreted simply as the probability of the fact that in the space preceding the first obstacle (however long it is), no nuclei form in the time t. If the behavior of $J(t)$ at $t \longrightarrow \infty$ is such that the integral

$$I_\infty = \int_0^\infty dt J(t)$$

converges, i.e., $J(t)$ decreases faster than t^μ at $\mu < -1$, $Q(t) \longrightarrow Q_\infty = n/(n + I_\infty)$ at $t \longrightarrow \infty$, and the final fraction of the initial phase $[n/(n + I_\infty)]^2$ is preserved indefinitely, i.e., the transformation is incomplete.

To calculate the average transition time from (23), we obtain

$$t_{av} \approx \int_0^\infty dt \left[\frac{n}{n + I(t)}\right]^2. \quad (24)$$

Hence, if $J(t)$ decreases similar to t^μ at $-1 < \mu \leq -1/2$, then the transformation is complete but takes an infinite amount of time, while at $\mu > -1/2$ complete transformation occurs in a finite amount of time. Calculation of the average transition time with the transformation kinetics determined by expression (22) yields a function varying with increasing n from t_{av0} (2) to t_{av} (24). This function is illustrated in Fig. 3 (curve 7).

If $J(t) = J_\mu t^\mu$ in the entire region of variation in t, integral (24) is calculated in the explicit form and yields at $\mu > -1/2$

$$t_{av} = \left(\frac{n}{J_\mu}\right)^{1/(\mu+1)} \frac{\mu}{(\mu+1)^{(1+2\mu)/(1+\mu)}} \times \frac{\pi}{\sin[\pi/(\mu+1)]}. \quad (25)$$

At $\mu \longrightarrow -1/2$, the average transformation time tends to infinity according to the law

$$t_{av} \longrightarrow \left(\frac{n}{J_{-1/2}}\right)^2 \frac{1}{8(\mu + 1/2)}.$$

5. PROBABILITY OF THE PRESERVATION OF FINITE INTERVALS OF THE INITIAL PHASE

Now, we pass to description of the spatial pattern of the transformation. First of all, we calculate the size distribution of the time-decreasing interdomain spacings. The probability of the fact that on either side of the specified point, e.g., to the right, a spacing with the length l_1 is not trapped by the new phase domain created on this side by the time t can be written as the product of the probability $\exp[-l_1 I(t)]$ of the fact that a nucleus does not form on the length l_1 in the time t and the probability $Q(t)$ of the fact that the spacing boundary is not trapped by the domain created on the right of it by the time t. This product is $\exp[-l_1 I(t)]Q(t)$. Differentiating it according to l_1, we arrive at the probability of having a free spacing with a length from l_1 to $l_1 + dl_1$ on the right in the form $I(t)\exp[-l_1 I(t)]Q(t)dl_1$ (similarly, on the left for a spacing from l_2 to $l_2 + dl_2$). The density of the probability that this point belongs to a spacing with a length from l to $l + dl$ for any l_1 and l_2 is

$$p_1(l) = \int_0^\infty dl_1 \int_0^\infty dl_2 \delta(l_1 + l_2 - l) I(t)^2 \times \exp[-I(t)(l_1 + l_2)]Q^2(t) = I(t)^2 l \exp[-lI(t)]Q^2(t). \quad (26)$$

Note that the probability that this point belongs to any free spacing is equal to the integral of $p_1(l)$ over all l, which, as can be easily seen, yields $Q^2(t)$, i.e., simply a fraction of the initial phase, as it must be.

Let us find the density of the distribution of free spacings between the initial phase domains of a specified size per unit system length. The calculation scheme used below makes the transition from the function $p_1(l)$ to the desired quantity simpler than in the approaches described in available publications.

We divide the spacing l into cells of small length Δl. The number of cells in this spacing is $n \approx l/\delta l$. The probability that a specified cell belongs to a free spacing of n cells is $p_1(l)\Delta l$. Let the system length be $L \approx N\Delta l$. We calculate the total number of free spacings of n cells on this length. If we multiply the probability $p_1(l)\Delta l$ by N, then each spacing will be taken into account in $Np_1(l)\Delta l$ for as many times as the number of cells in it. Therefore, the number of different spacings is obtained by dividing $Np_1(l)\Delta l$ by n. As a result, we obtain $N_l = (N/n)p_1(l)\Delta l$. To find the number of such spacings per system unit length, we divide N_l by L. Then, we have $I(t)^2\exp[-I(t)l]Q^2(t)\Delta l$, i.e., returning to the continual description, the probability of finding a free spacing with a length from l to $l + dl$ per unit length is

$$p(l)dl = I(t)^2 \exp[-lI(t)]Q^2(t)dl. \quad (27)$$

The total density of free spacings of all lengths is determined by integrating over l: $g = I(t)Q^2(t)$. Since each free spacing is limited by two boundaries (we assume the left boundary to be a kink and the right boundary to be an antikink), quantity g yields also the density of the number of domain walls with the same sign (or topological charge). The time evolution of the domain-wall density in the system is illustrated in Fig. 4a.

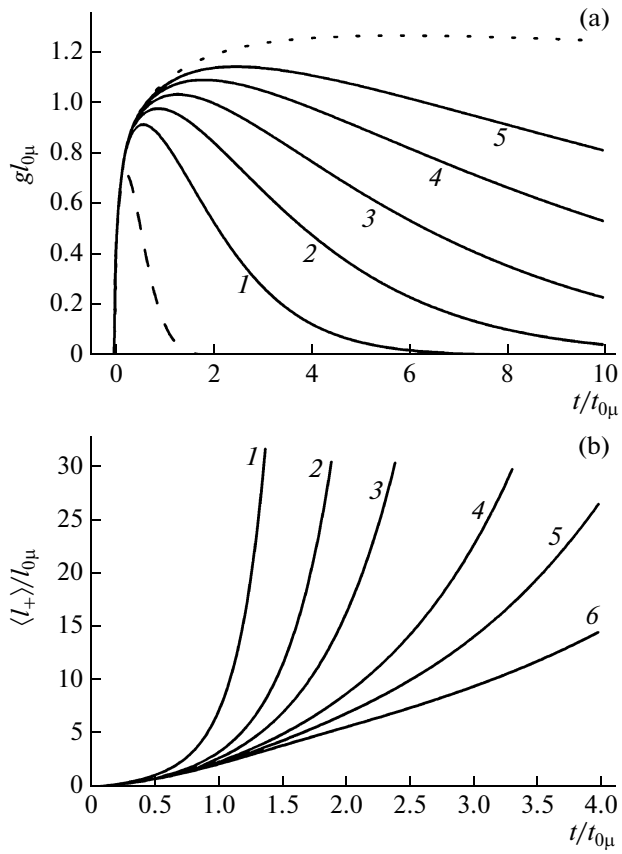

Fig. 4. (a) Kink (antikink) density evolution for delay times $\tau/t_{0\mu}$ of (*1*) 1, (*2*) 2.5, (*3*) 5, (*4*) 10, (*5*) 20 ($\mu = -1/2$ and $n = 5n_{0\mu}$). (b) Evolution of the average length of the new phase domains without (curve *1*) and with defects for average times of domain-wall delay at them $\tau/t_{0\mu}$ of (*2*) 0.5, (*3*) 1, (*4*) 2, (*5*) 3, and (*6*) 5 ($\mu = -1/2$ and $n/n_{0\mu}$).

The probability of finding a free spacing with a length from l to $l + dl$ normalized to unity is $p(l)dl/g = I(t)\exp[-lI(t)]dl$. Then, the average free-spacing length is

$$\langle l_-\rangle = \int_0^\infty I(t)\exp[-I(t)l]ldl = 1/I(t). \quad (28)$$

Free spacings alternate with occupied ones and, on average, the length of such a pair $\langle l_-\rangle + \langle l_+\rangle$ is equal to the average distance between the free spacings (e.g., between their left boundaries, i.e., kinks) $1/g = 1/[I(t)Q^2(t)]$. Thus, we find the time variation in the average size of the new phase domain

$$\langle l_-\rangle = 1/[I(t)Q^2(t)] - 1/I(t). \quad (29)$$

The time evolution of the average length of the new phase domains described by Eq. (29) is illustrated in Fig. 4b for several values of the defect density. One can see fast growth of the average domain size with time at the domain-coalescence stage. This growth becomes slower as the density of defects increases.

6. CONCLUSIONS

The theory developed in this study describes the space-time kinetics of the phase transformation of one-dimensional systems of a different nature with chaotically distributed defects hindering domain-wall motion. An equation was derived and analyzed that yields a statistical description of the time dependence of a transformed substance fraction. Taking into account the effect of defects, this equation generalizes the result of the Kolmogorov–Johnson–Mehl theory. The proposed theory allows calculation of the modification of the evolution of the initial-phase spacing distribution and the average size of the new phase domains caused by defects as a function of the defect density, average delay of domain motion due to them, and other parameters of the problem. It was shown that the effect of defects can lead to the occurrence of such qualitatively different kinetic types as incomplete transformation with the former phase preserved, complete transformation in an infinite amount of time, and complete transformation in a finite amount of time. As applied to DNA molecule replication, such classification of the modes can be useful for estimating the effect of defects on the life cycle of a cell [3, 20].

In study [27] devoted to the crystallization kinetics of amorphous Se and Se:Te alloy, it was established that the crystallization mechanism was uniform one-dimensional growth, which can be described, in a certain approximation, within the Kolmogorov–Johnson–Mehl model. It was demonstrated that doping with Te atoms significantly slows the growth of conductivity of the material upon its transition to the crystal state. This experimental fact can be qualitatively explained by the hindering of coalescence of the domains of a new, high-conductivity crystal phase by foreign atoms, as predicted in this study.

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