

Nanosized levels of the self-organized structures in the non-crystalline semiconductors As–S(Se) system

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Abstract. A synergetic model of the transition to a non-crystalline state is proposed, which enables us to investigate the temperature dependence of the microscopic parameters (mean-square displacements, the proportion of atoms in soft atomic configurations, power constants) under the influence of the external control parameter – the cooling velocity. Their analysis has been performed on the basis of experimental researches for non-crystalline semiconductors of the system As–S(Se). It has been shown that formation of self-organized structures in the non-crystalline solids is carried out in accordance with the technological conditions of obtaining as a method of the system self-organization. The dependence of the period and lifetime of self-organized structures on the cooling velocity has been studied. The established value of the period of spatial inhomogeneity $L_c \approx 10 \dots 10^2 \text{ \AA}$ correlates with the nanosized middle order in non-crystalline materials of the system As–S(Se) and decreases with increasing the cooling velocity.

Keywords: fractality, non-crystalline semiconductors, self-organized structures, synergetics, three-dimensional bifurcation diagram.

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1. Introduction

Non-crystalline semiconductor materials are fruitful and unique objects of practical and fundamental applications [1-5]. This is primarily correlated with the technological conditions of their preparation, the possibility of a wide variation of structural-sensitive parameters, the search for new areas of application [3-6]. The direction of semiconductor structures development with complementarity properties of nanocomposite materials and synergy of energy saving technologies with the corresponding implementation of anticipated structural-sensitive properties is extremely important and relevant [4, 7, 8]. In addition, physics of self-organization processes in non-crystalline systems is not isolated or unitary, but, on the contrary, represents only a part of a rather broad class of analogous phenomena in open systems [8-10]. The ideas that underlie the concept of self-organization processes in non-crystalline solids proved to be quite fruitful, and today they have wide practical application both in physics of semiconductors [9, 11], as well as in adjacent fields – physics of biocompatible media, materials of the artificial intelligence and information technologies [5, 11-14].

The paper presents synergetic effect of obtaining semiconductor materials with formation of self-organized structures. The aim of this research was to establish the regularities of forming the self-organized structures and corresponding realization of anticipated structural-sensitive properties, to determine their functional parameters, in particular nanosized levels of structuring and lifetime, to compare the results with known empirical relationships.

2. Formation of the self-organized structures in the non-crystalline systems

2.1. Concepts and investigation methods

Let us consider the system and corresponding conditions for obtaining non-crystalline semiconductor materials by cooling the melt [1, 2]. In a non-equilibrium non-crystalline system (NCS) for a non-adiabatic process in which non-crystalline materials are produced, the amount of heat dQ from the environment (thermostat) is equal $dQ = TdS$ [8, 15]. In this case, it is necessary to consider the flow of negative entropy from the surrounding environment $dS_e = f(q) \leq 0$, where q is the external control parameter, which is defined by the velocity of

change in temperature. The kinetics of temperature changes $\frac{dT}{dt}$ for the system is determined by an equation that takes into account the processes of heat conduction and heat exchange:

$$\rho \cdot C \frac{\partial T}{\partial t} = \text{div}(\chi \cdot \text{grad}T) - Q(T), \quad (1)$$

where C , ρ , and χ are heat capacity, density and thermal conductivity of the system, $Q(T)$ is heat-exchange with the environment with a heat-transfer coefficient η_h . Initial and boundary conditions:

$$T(r, z, t)|_{t=0} = T_0, \quad T(r, z, t)|_{r=r_0} = T_0,$$

$$T(r, z, t)|_{z=0, d} = T_0,$$

$$\chi \frac{\partial T(r, z, t)}{\partial z} \Big|_{z=0} = \eta_h (T(r, z, t) - T_{TS}(r, z, t)) \Big|_{z=0},$$

$$\chi \frac{\partial T(r, z, t)}{\partial r} \Big|_{r_0=0} = \eta_h (T(r, z, t) - T_{TS}(r, z, t)) \Big|_{r_0=0}.$$

It is taken into account that the sample of NCS materials in the form of a cylindrical rod with a radius r_0 and length d is located along the axis z , the temperature of the thermostat is T_{TS} . Obtaining the materials of NCS by cooling the rinse is a complex of physical-and-chemical processes that occur in highly non-equilibrium conditions [1-3]. The non-equilibrium conditions of the system are caused by the temperature gradient between the cooled surface and the surrounding environment (the thermostat). The transition to a non-crystalline state occurs at cooling speeds of the system $q = \frac{dT}{dt} \geq q_c$, where q_c is the limiting cooling speed, under which in the system no germ cell capable of crystalline phase is formed. According to the Arrhenius ratio [7], the period of formation of a crystalline nucleus is the characteristic value

$$\tau = \tau_0 \exp\left(\frac{L_a}{RT}\right), \quad (2)$$

where the activation energy of crystallization is L_a , the universal gas constant is R [1]. Having differentiated the left and right sides in the ratio (2) in time, we obtain

$$\frac{dT}{dt} = \frac{1}{\tau_0} \frac{RT^2}{L_a} \exp\left(-\frac{L_a}{RT}\right).$$

The limit cooling speed can be defined as the limiting velocity at the crystallization temperature $T = T_m$ and is equal

$$q_c = \frac{RT_m^2}{\tau_0 L_a} \exp\left(-\frac{L_a}{RT_m}\right). \quad (3)$$

The temperature distribution $T(r, z)$ and the speed of its change $T(r, z)/dt$ can be obtained according to Eq. (1) by using numerical methods taking into account the thermophysical characteristics of the material and the specific heat transfer conditions that correspond to the glass production method, as well as the values of the technological parameters of the quenching process and the sizes of the received material NCS. The calculation is considerably complicated when taking into account the condition of the cooled surface (the presence of random contaminants or oxides), which affects the heat transfer process [3]. The influence of the relevant factors can be taken into account in the introduction of the theoretical consideration of the phenomenological heat-transfer coefficient η_h , which is determined on the basis of experimental studies under different technological conditions of production and is a certain characteristic for the chosen method of obtaining a range of values [2, 11].

Using the definition of the coefficient of thermal conductivity $a_T = \frac{\chi}{\rho C}$, the reduced coefficient of heat-

transfer $a_\eta = \frac{\eta_h}{\rho C d}$, in the one-mode approximation [7]

we rewrite the equation (1) as follows:

$$\frac{\partial T}{\partial t} = -a_T \frac{T}{L_\chi^2} + a_\eta (T_{TS} - T).$$

Here, L_χ is the characteristic scale of thermal conductivity.

The characteristic time intervals of temperature changes in the cooling system satisfy inequalities

$t_T \ll t_{\text{exp}}$, where $t_T = \frac{L_\chi^2}{a_T}$ is the characteristic time of

change in temperature that is due to the temperature conductivity. According to the definition of kinematic

viscosity $\nu = \frac{\eta_{\text{visc}}}{\rho}$ and determining the time of

relaxation of the state of the system $t_{\text{rel}} = \frac{\eta_{\text{visc}}}{G}$ and the

velocity of sound $S_f = \sqrt{\frac{z f a_0^2}{2M}} = \sqrt{\frac{G}{\rho}}$, where η_{visc} is the

viscosity, G is the shift modulus, the condition $t_T \ll t_{\text{exp}}$

and $t_{\text{rel}} \approx t_{\text{exp}}$ takes the form $a_T t_T \ll \frac{a_T \nu}{S_f^2}$. Since the

spatial dimension of the thermal conductivity is characteristic

$L_\chi = \sqrt{a_T t_T}$, then the condition $t_T \ll t_{\text{exp}}$ means that L_χ should be smaller than the value

$L = \frac{\sqrt{a_T \nu}}{S_f}$. The physical content of this inequality

is expressed in hydrodynamic equation $t_T t_\epsilon \omega_k^2 \ll 1$,

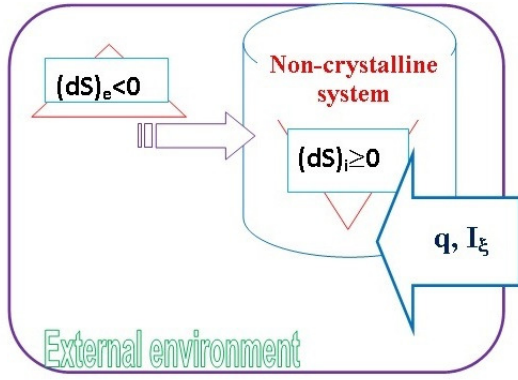


Fig. 1. Formation of a non-crystalline state (external control parameters are the cooling velocity q and obtaining conditions I_ξ).

according to which the value of the product of the time of heat conduction t_T and convection t_e is much smaller than the square of the inverse frequency of the sound ω_k (here, it was taken into account that $kL \approx 1$, $\tau_e^{-1} = vk^2$, $\omega_k \approx S_f k$, $\tau_{rel} \tau_e \omega_k^2 = 1$ and the wave vector is k). For the non-crystalline solids of the system As–S(Se) with characteristic values of parameters ($S_f \approx 10^5$ cm/s, $\rho \approx 3 \dots 4.5$ g·cm $^{-3}$, $C \approx 0.5 \dots 0.9$ J·g $^{-1}$ ·K $^{-1}$, $\chi \approx 10^{-3} \dots 10^{-2}$ W/(K·cm), $v \approx 10^{11} \dots 10^{14}$ cm 2 /s, $\eta_h \approx 10^{-3} \dots 10^{-2}$ W/(cm 2 ·K), $a_T \approx 2.4 \cdot 10^{-4} \dots 6 \cdot 10^{-2}$ cm 2 /s [1-5]) we get $\frac{L_\chi}{L} \approx 10^{-3} \dots 10^{-2}$. Consequently, the condition $\frac{L_\chi}{L} \ll 1$ is fulfilled for the non-crystalline solids [6, 11, 17].

2.2. Synergetics approach

For the non-crystalline system in contact with the thermostat, statistical averages describing the system in this state can be obtained in the framework of the concept of non-equilibrium statistical operator [8]. It should be noted that the free energy, entropy of the NCS state are not state functions (as in the equilibrium case), since they depend on the external control parameter q (Fig. 1, $(dS)_e$ is an entropy flux that exists due to exchange a mass, energy and information with the environment, and $(dS)_i$ is an entropy production inside the system).

But, at the same time, as shown by Haken ([8, 10]), they can be used to describe the behavior of strongly non-equilibrium systems, in particular dependence on q , based on a formal analogy between non-equilibrium transformations and second-order phase transitions [13-15]. We will analyze the kinetics of changing the system parameters, namely, the proportion of atoms in soft configurations σ and the reduced mean-square displacements along the bond $y_l = 36D_l^{\alpha\alpha}/r^2$ and perpendicular to it $y_t = 4D_t^{\alpha\alpha}/r^2$ (r is the interatomic

distance) in a strongly non-equilibrium conditions (the expediency and adequacy of the application of these values is analyzed in detail by the authors [14, 15]). The parameters of the system σ , y_l , y_t determine the behavior of structural-sensitive properties of the NCS materials: modulus of shift ($\approx y_l$), deformation values ($\approx y_t$), and middle order ($\approx \sigma$). Having expanded F in degrees of system deviation from equilibrium and limited to the first members of the schedule, we have:

$$F = F_0 + \frac{1}{2} \sum_{i,j} a_{ij} \eta_i \eta_j + \frac{1}{3} \sum_{i,j,k} c_{ijk} \eta_i \eta_j \eta_k + \frac{1}{4} \sum_{i,j,k,l} b_{ijkl} \eta_i \eta_j \eta_k \eta_l, \quad (4)$$

where such notation is introduced:

$$\eta = \sigma - \sigma_e, \quad \eta_{y_l} = y_l - y_l|_e, \quad \eta_{y_t} = y_t - y_t|_e, \\ a_{ij} = \left(\frac{\partial^2 F}{\partial \eta_i \partial \eta_j} \right)_e, \quad c_{ijk} = \frac{1}{2} \left(\frac{\partial^3 F}{\partial \eta_i \partial \eta_j \partial \eta_k} \right)_e, \\ b_{ijkl} = \frac{1}{6} \left(\frac{\partial^4 F}{\partial \eta_i \partial \eta_j \partial \eta_k \partial \eta_l} \right)_e, \text{ and it is taken into account}$$

that $\left(\frac{\partial F}{\partial \eta_i} \right)_e = 0$ (index “e” corresponds to the equilibrium state). Since, as the numerical analysis shows, the quadratic and higher order terms of decomposition F by η_y are insignificant ($\approx 10^{-6} \dots 10^{-9}$) as compared with η^3 ($\approx 10^{-2}$) and η^4 ($\approx 10^{-3}$), then in the expansion (4) we can limit the quadratic by η_{y_l} and η_{y_t} terms:

$$F = F_0 + \frac{1}{2} \sum_{i,j} a_{ij} \eta_i \eta_j + \frac{c}{3} \eta^3 + \frac{b}{4} \eta^4. \quad (5)$$

Here, $c = \frac{1}{2} \left(\frac{\partial^3 F}{\partial \eta^3} \right)_e$, $b = \frac{1}{6} \left(\frac{\partial^4 F}{\partial \eta^4} \right)_e$. Based on (5), we get:

$$\frac{\partial F}{\partial \sigma} = a_{11} \eta + a_{12} \eta_{y_l} + a_{13} \eta_{y_t} + c \eta^2 + b \eta^3, \\ \frac{\partial F}{\partial \eta_{y_l}} = a_{12} \eta + a_{22} \eta_{y_l} + a_{23} \eta_{y_t}, \\ \frac{\partial F}{\partial \eta_{y_t}} = a_{13} \eta + a_{23} \eta_{y_l} + a_{33} \eta_{y_t}. \quad (6)$$

For the purpose to describe the kinetics of changes in order parameters, we use the Landau–Khalatnikov equation [8, 10]

$$\frac{\partial \eta_i}{\partial t} = -\gamma_i \left(\frac{\partial F}{\partial \eta_i} \right),$$

which allows one to shift in the relations (6) to the following system of nonlinear kinetic equations:

$$\begin{aligned} \gamma_1 \frac{\partial \eta}{\partial t} &= -a_{11}\eta - a_{12}\eta_y - a_{13}\eta_\Phi - c\eta^2 - b\eta^3, \\ \gamma_2 \frac{\partial \eta_{y_l}}{\partial t} &= -a_{12}\eta - a_{22}\eta_{y_l} - a_{23}\eta_{y_t}, \\ \gamma_3 \frac{\partial \eta_{y_t}}{\partial t} &= -a_{13}\eta - a_{23}\eta_{y_l} - a_{33}\eta_{y_t}. \end{aligned} \quad (7)$$

The first terms in equations (7) describe the dissipative process of relaxation of the fraction of atoms in the soft configurations, deformation and shift to equilibrium state with the relaxation time $\tau_{ij} = a_{ij}^{-1}$, and the second terms determine the process of interaction of collective modes. We use the principle of the hierarchy of time scales [10, 15] and subordination of the modes of Prigozhin to strongly nonequilibrium systems [8]. The characteristic time intervals for changing the field of deformation and the interatomic distance of the system during the cooling process satisfy the inequalities $t_{y_l} \ll t_{\text{exp}}$, $t_{y_t} \ll t_{\text{exp}}$, and $t_{\text{rel}} \approx t_{\text{exp}}$, $t_{y_l}, t_{y_t} \leq t_{\text{loc}}$ and, always, are fulfilled, since $t_{y_l}, t_{y_t} \approx 10^{-12}$ s [16]. Taking into account the above estimates, we can approximate it

$$\frac{\partial \eta_{y_l}}{\partial t} \approx 0, \quad \frac{\partial \eta_{y_t}}{\partial t} \approx 0, \quad \frac{\partial T}{\partial t} \approx 0.$$

This allows you to reduce the number of order parameters:

$$\begin{aligned} \eta_{y_l} &\approx -\left(\frac{a_{23}a_{13} - a_{12}a_{23}}{a_{22}a_{33} - a_{23}^2} \right) \eta, \\ \eta_{y_t} &\approx -\left(\frac{a_{13}a_{22} - a_{12}a_{23}}{a_{23}^2 - a_{33}a_{22}} \right) \eta, \quad T \approx \frac{T_{TS}}{\frac{a_T}{L_\chi^2} + a_\eta} \end{aligned}$$

and consider the temperature field, the fields of deformation and the shift of atoms self-consistent with the field of distribution in soft atomic configurations. Hence, we can write (7) in the form

$$\gamma_1 \frac{\partial \eta}{\partial t} = -a_0\eta - c\eta^2 - b\eta^3, \quad a_0 = -\left(a_{11}^2 - \frac{a_{12}^2}{a_{22}^2} - \frac{a_{13}^2}{a_{33}^2} \right).$$

We will restrict ourselves to this section by considering the external controlling parameter, it is the cooling velocity: $dS_e = f(q)$ (Fig. 1). Then, the coefficients of decomposition are functions of temperature, pressure and control parameter, the cooling velocity: $a_0 = a_0(T, P, q)$. Since it is in equilibrium

$$\delta F = 0, \quad dS_e = 0, \quad \delta^2 F > 0, \quad \text{and} \quad \eta = 0.$$

Then, in order to make this, the coefficient $a_0(T, P, q)$ should be positive, i.e., $a_0(T, P, q) > 0$. In a non-equilibrium state

$$\delta F \neq 0, \quad dS_e \leq 0, \quad \eta \neq 0 \quad \text{and} \quad a_0(T, P, q) < 0.$$

Stationary states with non-zero order parameter

$$\eta = \frac{-2c \pm \sqrt{4c^2 - 4a_0b}}{6b}$$

are implemented with $a_0(T, P, q) < 0$. Consequently, when transitioning to a non-equilibrium state with a non-zero parameter of order, the decomposition factor $a_0(T_c, P_c, q_c) = 0$. The following conditions should be also fulfilled: $c(T_c, P_c, q_c) = 0, b(T_c, P_c, q_c) > 0$, as if approaching a point T_c, P_c, q_c from the equilibrium state should be a positively defined form of the second derivative. Thus, in the process of cooling the melt and in the transition to a non-crystalline state, the value $a_0(T_c, P_c, q_c)$ can be approximated by the expression:

$$a_0(T_c, P_c, q_c) = -\tilde{a}_0 \cdot \arctan(\ln(\tilde{q})), \quad \tilde{q} = \frac{q - q_c}{q_c}, \quad (8)$$

which goes into $a_0(T_c, P_c, q_c) \approx -a_0\tilde{q}$ at $\tilde{q} \ll 1$. In (8), we use the reduced critical velocity \tilde{q} , which is determined from the condition (3) and depends on the characteristics of the system, in particular the nature of the interatomic interaction. The main emphasis in the proposed approach is on the common features of the transition to a non-crystalline state, namely, the study of the effect of non-equilibrium on the formation of non-uniform structures. For this purpose, considered is the given velocity \tilde{q} , which does not depend on the type of chemical bond.

3. Three-dimensional bifurcation diagram and branching of solutions

Hence, on the basis of the relations (1)–(8), we obtain the following self-consistent system of equations with respect to the fraction of atoms in soft atomic configurations σ , the mean-square displacements $y_l (D_l^{\alpha\alpha})$ and $y_t (D_t^{\alpha\alpha})$:

$$\begin{aligned} F_1(\sigma) &= -\tilde{a}_0\tilde{q}\eta + c\eta^2 + b\eta^3, \quad F_2(y_l) = \frac{\eta_{y_l}}{\tau_{y_l}}, \\ F_3(y_t) &= \frac{\eta_{y_t}}{\tau_{y_t}}. \end{aligned} \quad (9)$$

Here, the functions $F_1(\sigma)$, $F_2(y_l)$, $F_3(y_l)$ are defined according to the equations [9, 15]

$$F_1(\sigma) = \sigma \xi_P + (1 - \sigma) z \left\{ \frac{e^{-y_l} \left[B(y_l) - \frac{P^* e^{y_l}}{12(1 - \sigma)^2} \left(\frac{r}{a_0} \right)^2 \right] + \frac{G_0/V_0}{(1 + 2y_l)}}{2} \right\} -$$

$$- z(1 - \sigma) \sigma \left(1 + \frac{y_l}{4} - \frac{1}{6} \ln \frac{B(y_l)}{2} \right) A(y_l) -$$

$$\tau \ln \frac{\frac{g_2 - 1}{\sigma}}{\frac{g_1 - 1}{1 - \sigma}} = 0. \quad (10)$$

$$F_2(y_l) = \frac{3e^{-y_l} \tau}{8\sqrt{2}(1 - \sigma)} \left[B(y_l) + \frac{P^* e^{y_l}}{6(1 - \sigma)^2} \right]^2 \times$$

$$\times \left(1 + \frac{0.022(1 + 2y_l)^{-2}}{e^{y_l} \left[B(y_l) + \frac{P^* e^{y_l}}{6(1 - \sigma)^2} \left(\frac{r}{a_0} \right)^2 \right]} \right) - y_l = 0,$$

$$F_3(y_l) = \frac{3(1 + 2y_l) \tau}{8(1 - \sigma) e^{\frac{y_l}{2}}} \left[B(y_l) + \frac{P^* e^{y_l}}{6(1 - \sigma)^2} \left(\frac{r}{a_0} \right)^2 \right]^{\frac{1}{2}} -$$

$$- y_l = 0. \quad (11)$$

Here, $\tau = \theta/V_0$ is the reduced temperature, $\xi_P = \phi/V_0$, G_0/V_0 are the parameter of the anisotropy of the potentials. This self-consistent system of equations (9)–(11) makes it possible to investigate the dynamic stability and temperature behavior of the system under non-equilibrium phase transformations ($q \neq 0$), by using the calculation results obtained for equilibrium transformations ($q = 0$).

The solution of the resulting system of equations (9)–(11) is carried out numerically using the iterative procedure and object-oriented modeling [14]. The results of calculations are presented in Fig. 2 in the case of different cooling velocity. We will analyze the peculiarities of changing the dynamic stability of the system with the change of the external control parameter – the cooling velocity q , in particular with $\tilde{q} \rightarrow \tilde{q}_c$. Solutions of the system of equations for the proportion of atoms in the soft configurations and the mean-square displacements of atoms have, at one value of the control parameter and the temperature, at least two stable states that differ in the degree of dynamic stability and ordering (Fig. 2). The first region covers the state of the system at cooling speeds $\tilde{q} < \tilde{q}_c$, which contains the transition from a dynamically unstable to a dynamically stable solid

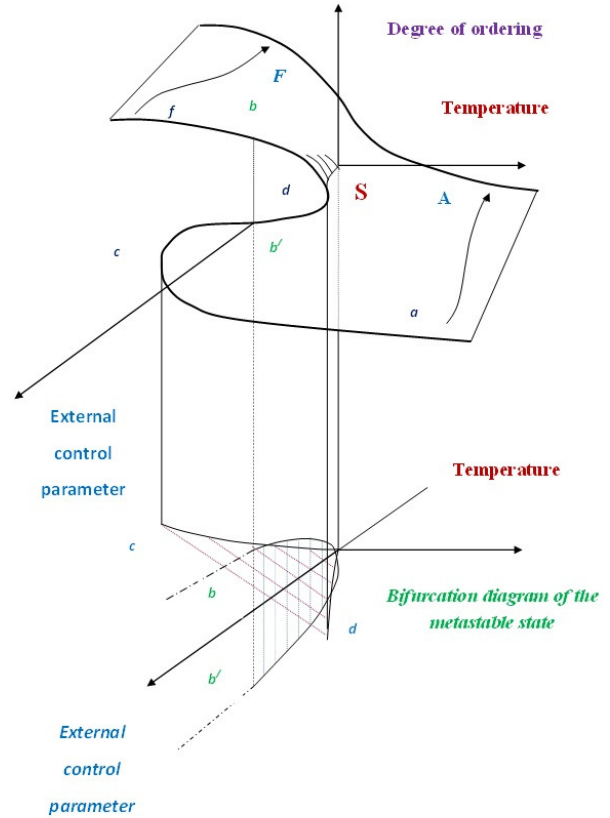


Fig. 2. Branching of the solutions of the characteristic equation at different of the external control parameter q .

(crystalline, quasi-crystalline) state and is accompanied by an abnormal increase in elastic constants with simultaneously abrupt decrease in the atomic fraction in soft atomic configurations and the amplitude of the mean-square displacement at lowering the temperature.

As can be seen from Fig. 2, the degree of statistical disordering in a solid increases with $\tilde{q} \rightarrow \tilde{q}_c$ (a sharp change is observed in the transition to a quasi-crystalline state on the part of the metastable state, a supercooled liquid) and, thus, increases the temperature transition interval of the supercooled liquid. A quasi-linear dependence of the system parameters in the considered change interval for a dynamically stable crystalline branch is observed (Fig. 2, branch *a-b*). At $\tilde{q} < \tilde{q}_c$ in the region of transition temperatures $\tau = \tau_m$, the proportion of atoms in soft atomic configurations and the mean-square displacements of atoms vary jump-like (the value of this change decreases with the growth of \tilde{q}). Consequently, the macroscopic properties of the system are in proportion to σ , y_l (for example volume), and their derivatives $\sigma'(\tau)$, $y_l'(\tau)$ (for example, the coefficient of linear expansion, heat capacity) have an anomaly at $\tilde{q} \rightarrow \tilde{q}_c$. The second region, which is realized at $\tilde{q} > \tilde{q}_c$, is characterized by a continuous anomalous increase in the stiffness of the frame and elastic constants, a continuous decrease of σ , y_l with a decrease in temperature (Fig. 2). So, the curve $\sigma(\tau, \tilde{q})$ at $\tilde{q} = \tilde{q}_c$

delimits in the temperature range $\tau \geq \tau_c$ the existence of metastable supercooled liquid and a dynamically stable non-crystalline system. It determines the lower boundary of the potential in the temperature range from τ_0 before τ_c to cooling $\tilde{q} < \tilde{q}_c$ (τ_0 is the synthesis temperature) of the existence of a supercooled state. The temperature τ_c on the curve $\sigma(\tau, \tilde{q})|_{\tilde{q}=\tilde{q}_c}$ (for which the metastable states degenerate) is the coexistence temperature at a given pressure of three states, crystalline, liquid, and non-crystalline: $\left(\frac{\partial^2 \sigma}{\partial \tau^2}\right)_{\tau_c} = 0$.

Investigation of the behavior of thermodynamic properties in the system in the vicinity $\{\tau_c, q_c\}$ causes separate interest. It should be noted that the correlated decrease in the intensity of atomic oscillations, their amplitudes and the growth of the elastic constants in the transition from the metastable supercooled melt to the non-crystalline solid state indicates the presence of macroscopic processes at the level of microstructural

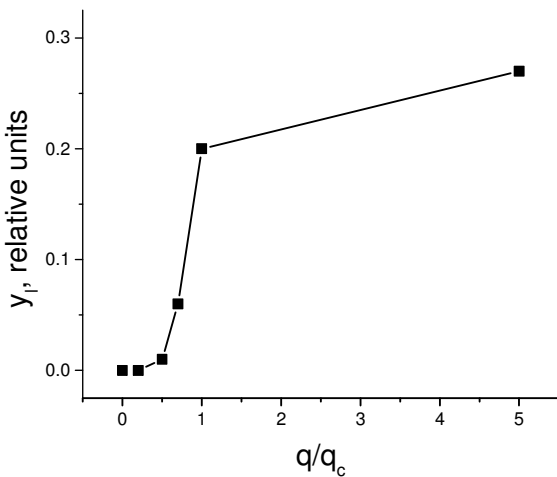


Fig. 3. Bifurcation dependence of the reduced mean-square displacement of atoms y_l at temperature $\tau = 0.1$ on the cooling speed q/q_c .

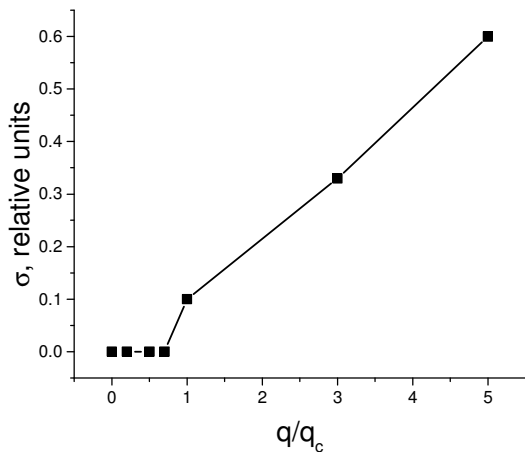


Fig. 4. Bifurcation dependence of the fraction of atoms in configurations σ at temperature $\tau = 0.1$ on the cooling speed q/q_c .

rearrangement, for which, in accordance with the values of the control parameter \tilde{q} , a non-crystalline structure with a parameter of ordering η takes place. The order parameter that we use is determined by the spontaneous appearance of non-zero values of the displacement module and depends on the degree of system deviation from the equilibrium state (Figs. 3, 4). The structure formed at $\tilde{q} > \tilde{q}_c$ is the result of the loss of the dynamic stability in the basic equilibrium state, when the temperature in the region decreases $\tau \leq \tau_m$. This structure arises due to the self-consistent amplification of fluctuations (mean-square displacements of atoms, their fraction in soft atomic configurations) that reach the mesoscopic level and make a stable new structure [15].

This method of organizing the structure corresponds to and defines self-organized structures. Formation of a self-organized structure in non-crystalline solids, when cooling the system, is due to self-consistent creation of regions of soft atomic configurations and the temperature behavior of structural-sensitive characteristics that correspond to the minimum energy dissipation for given external parameters, cooling speed and technological regimes of obtaining [14]. This circumstance is essential for a non-crystalline system and allows the non-crystalline structure to be determined through self-organization. Under self-organization, in this case, the macroscopic manifestation of processes occurring at the microscopic level, the fields of dynamic and static displacements of atoms, is understood, which causes spontaneous formation of the non-zero component of shift module (Fig. 4). It should be emphasized that the nature of the dependence of the degree of disordering in non-crystalline solids on \tilde{q} correlates with the change of elastic constants at a given temperature, when their growth \tilde{q} decreases and the framework of the material becomes more labile and capable of rearrangement under the influence of external factors [5, 9]. Formation of a self-organized structure in non-crystalline solids under cooling is related to the self-consistent creation of the “soft”-state domains and results from the temperature behavior of the structures under evolution towards those changes that may promote the minimum energy dissipation and facilitate the technological process. Functional organization of the very self-organized structure is also defined by the selected qualitative energy that is selected ordering from chaos. These methods are determined through external control parameters and form the appropriate types of ordering.

The transition to a non-crystalline state can be considered as a process of the self-organization with using the principles of synergetics [12, 19]. The choice of a nonlinear mathematical model of a dynamic object that is a non-crystalline system in the process of action of an external controlling parameter is reduced to a system of nonlinear equations. Based on the above, we will analyze the features of the qualitative behavior of the transition to a non-crystalline state, depending on the external control parameter – the cooling speed (Fig. 5). The presence of



Fig. 5. Obtaining of the non-crystalline materials as a self-organized process in an open system.

self-organization processes and formation of self-organized structures in the transition to a non-crystalline state involve a whole series of unique properties and states of semiconductor materials [14]. One this feature is nano-level structuring and fractality of lifetime.

4. Nanosized levels structuring of the self-organized structures

Let's analyze the influence of the nonlocal distribution of the order of the system parameter η . In this case, the equation (7) takes the form [17, 18]:

$$\frac{\partial \eta}{\partial t} = a_0 \arctan(\ln(1 + \tilde{q}))\eta - c\eta^2 - b\eta^3 + D \cdot \Delta \eta. \quad (12)$$

Here, D is the diffusion coefficient, Δ is Laplacian, which describes the diffusion type non-locality. The equation (12) is solved at the initial and boundary conditions for NCM in the form of a cylindrical rod with the radius r_0 and length d , located along the axis z . To find out the stability of the system, we consider infinitesimal perturbations of the solutions of the thermodynamic branch

$$\eta(r, t) = \eta_s + \delta\eta(r, t). \quad (13)$$

Here, $\delta\eta(r, t)$ is a deviation of the system from a homogeneous stationary state η_s , caused by random fluctuations ($\delta\eta(r, t) \ll 1$). Let's rewrite the term $\delta\eta(r, t)$ in the form of a Fourier series expansion:

$$\delta\eta(r, t) = \sum_k A \cdot \exp\{ikr + \lambda t\}. \quad (14)$$

Here, A is the amplitude mode with wave vector k and increment of attenuation λ .

Substituting (14) into (13) and linearizing on the small parameter $\delta\eta(r, t)$, taking into account (12), we obtain a dispersion equation that correlates the increment of damping with the wave vector:

$$\begin{aligned} \lambda &= \lambda(k, \tilde{q}), \\ \lambda(k, \tilde{q}) &= a_0 \arctan(\ln(1 + \tilde{q})) + \\ &+ 2c\eta_s + 3b\eta_s^3 - D \cdot k^2. \end{aligned} \quad (15)$$

For $k^2 < k_c^2 = \frac{a_0 \arctan(\ln(1 + \tilde{q})) - 2c\eta_s - 3b\eta_s^3}{D}$ the

increment of attenuation is $\lambda(k, \tilde{q}) = (k_c^2 - k^2) \cdot D > 0$, which indicates a divergence of mode with a wave vector k . A typical dependence of the increment of attenuation on the wave vector is shown in Fig. 6.

In order to prove the existence of new solutions $\eta(r, t) = \eta_s + \delta\eta(r, t)$ of the system of equations (9)–(11) at $q \geq q_c$, in addition to the linear analysis of the stability of solutions (13), it is necessary to analyze the complete nonlinear equations by using the condition of transversality. The condition of transversality in the case of simple eigenvalues of the characteristic equation (15) will be written in the form

$$\frac{d}{d\tilde{q}} \lambda(\tilde{q}) = \frac{1}{1 + \tilde{q}} \cdot \frac{a_0}{1 + \ln^2(1 + \tilde{q})}, \quad \left. \frac{d}{d\tilde{q}} \lambda(\tilde{q}) \right|_{q=q_c} = a_0 \neq 0.$$

Because $\frac{d\lambda}{d\tilde{q}} \neq 0$, then with $q = q_c$ the whole branch

$\lambda(\tilde{q})$ as a function of \tilde{q} crosses the axis \tilde{q} and branching into a supercritical region (Fig. 2). This condition is a confirmation of the conclusion that the obtained solutions $\eta(r, t) = \eta_s + \delta\eta(r, t)$ branch out of the supercritical region are stable at $q \geq q_c$ and they correspond to the heterogeneous distribution of atoms in soft configurations. In addition, the solutions η_s remain constant on the macroscopic scales under consideration, and the time dependence varies quite slowly on the scale of the development of instability [18].

On the function λ , the condition of slowness of the change in the time of the species is imposed $\lambda_s^{-1} \frac{\partial \lambda}{\partial t} \ll \lambda$, which amounts to a slight change λ_s^{-1} on the macroscopic scale (adiabatic approximation [18]).

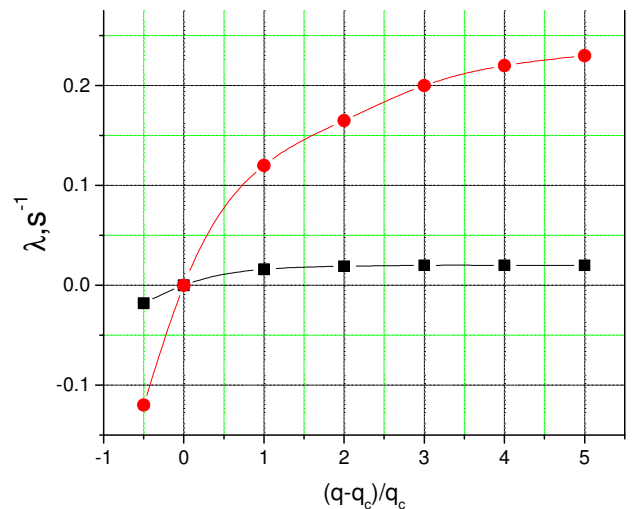


Fig. 6. Dependence of the attenuation increment λ from the reduced cooling speed \tilde{q} (● – $D = 10^{-15} \text{ cm}^2/\text{s}$, ■ – $D = 10^{-18} \text{ cm}^2/\text{s}$).

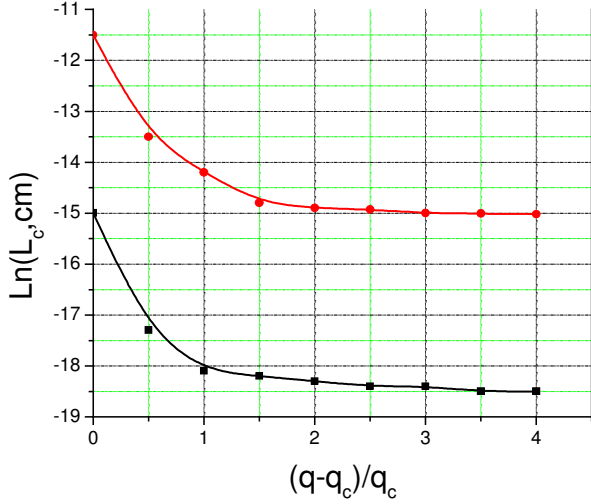


Fig. 7. Dependence of the period of the dissipative structure on the reduced cooling speed (● – $D = 10^{-15} \text{ cm}^2/\text{s}$, ■ – $D = 10^{-18} \text{ cm}^2/\text{s}$).

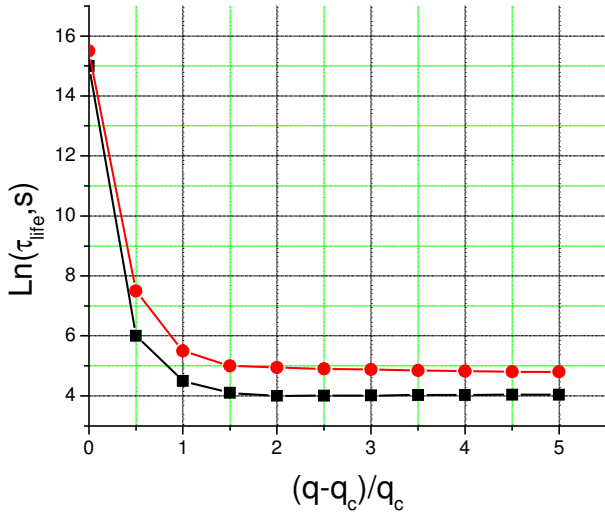


Fig. 8. Dependence of the lifetime of a self-organized structure for NCS on \tilde{q} (● – $a_0 = 0.1 \text{ s}^{-1}$, ■ – $a_0 = 0.2 \text{ s}^{-1}$).

The period and time of life of the formed dissipative structure depend on the control parameter \tilde{q} . At $\tilde{q} \rightarrow \tilde{q}_c$:

$$L_c = \frac{2\pi}{k_c} \rightarrow 2\pi \sqrt{\frac{D}{a_0 \arctan(\text{Ln}(1 + \tilde{q})) - 2c\eta_s - 3b\eta_s^2}},$$

$$\tau_{life} = \frac{1}{\lambda(\tilde{q}, k_c)} \rightarrow \frac{1}{a_0 \arctan(\text{Ln}(1 + \tilde{q})) - 2c\eta_s - 3b\eta_s^2}. \quad (16)$$

It should be noted that k_c is defined only by the system parameters. At $q > q_c$ above the point of instability of the thermodynamic state, k_c determines the spatial scale of heterogeneity of the stationary solution η_s . Thus, in a system that with $q < q_c$ was homogeneously stable, with values of the external control

parameter $q > q_c$ spontaneously generated its own scale of the ordering L_c (Fig. 7). Dependences of the heterogeneity period $\text{Ln}(L_c(\tilde{q}))$ and lifetime $\text{Ln}(\tau_{life}(\tilde{q}))$ in the self-organized structure of non-crystalline solids are given in Figs. 7 and 8. Size of the ordering period is $L_c \approx 10 \dots 10^2 \text{ \AA}$ and correlates with the nanosize of the middle order in the non-crystalline materials system As-S(Se) [14, 16]. In addition, lifetime is $\tau_{life}(\tilde{q}) \gg 1$.

5. Calculation results and empirical relations for the non-crystalline semiconductors

We analyze the change of the Debye–Waller parameter in the loss of the dynamic stability of the crystalline state and the transition to a non-crystalline state. Investigation of the temperature dependence of the cross-section of the dissipation of thermal neutrons by the melting of crystals and the non-crystalline solids allows obtaining microscopic data on the nature of the interatomic interaction and the peculiarities of the near and middle orders of these materials [5, 9]. Two times differentiated neutron scattering cross section σ_{DW} , attributed to the corpuscular element $d\Omega$ and the energy interval dE , is given by an expression [14, 20]

$$\frac{d^2\sigma_{DW}}{d\Omega dE} = \frac{1}{N} \delta(\hbar\omega) \sum_{i,j}^N a_i a_j \exp(-W_i) \cdot \exp(-W_j) \cdot f_{ij}(\tilde{\chi}), \quad (17)$$

where $\hbar\tilde{\chi} = \bar{P}_0 - \bar{P}$ and $\hbar\omega = E_0 - E$ are change of momentum and neutron energy during scattering, a_i is the scattering amplitude, $\exp(-W_i)$ is the Debye–Waller factor, $f_{ij}(\tilde{\chi}) = \exp(i\tilde{\chi}(\bar{R}_i - \bar{R}_j))$, \bar{R}_i – atomic coordinate.

Temperature dependence of σ_{DW} and $\exp(-W_i)$ for the crystalline state has a sharp decrease at the temperature of loss of dynamic stability, which is caused by the growth of intensity of atomic oscillations and restructuring the structure (a significant increase in the atomic share in soft atomic configurations σ and mean-square displacements y_b, y_l (relation (9), Figs. 2 to 4). Cooling the melt in conditions $q < q_c$ is accompanied by an increase in the scattering cross-section during the transition to a solid state, with the jump decreases with height q . At $q \geq q_c$ dependence σ_{DW} and $\exp(-W_i)$ on the temperature is monotonous. In the solid state, in the transition from crystal to non-crystalline solid at a given temperature, there is an increase in the amplitude of oscillations and static displacements, a decrease in the cross-section and intensity of scattering [21, 22].

The temperature behavior of the mean-square displacements of the atoms near the temperature of the loss of dynamic stability (Eq. (9), Figs. 2 and 3) is given by the expression [9, 14]

$$\sqrt{u^2} = \frac{r}{6} \left(1 + \frac{\Delta_s}{2} - (1 - T/T_s)^{1/2} \right)^{1/2}. \quad (18)$$

The resulting dynamic instability can be associated with the process of softening. It should be noted that the temperature dependence of the frequency of atomic oscillations in the vicinity T_s (when ω abnormally decreasing with $T \rightarrow T_s$ [14, 15]) corresponds to the experimentally observed temperature dependence of low frequency oscillations near the softening temperature T_g [21]. In addition, the temperature dependence of the reduced mean-square displacements $y(T)$ of non-crystalline materials at $T \rightarrow T_s$ (Fig. 2) correlates with the ratio obtained for the mean-square displacement by the authors of work [21] in the framework of the theory of bound modes:

$$\sqrt{u^2} = r \left(1 - \frac{a_r}{2} \sqrt{T_s - T} \right), \quad T \leq T_s, \quad (19)$$

and experimentally investigated for inelastic scattering of neutrons in glasses with van der Waals bond in the work [22]. This suggests a significant effect of the dynamic instability of the atoms in the process of softening NCS.

The type of chemical bond affects the limiting cooling rate q_c , at which the NCS material can be obtained as well as the degree of deviation from the state of equilibrium. So, for chalcogenide glass-like semiconductor system As–S(Se) the presence of directed covalent bonds, the polymeric structure determines the transition in the NCS with slight deviations from the equilibrium state and the values of the cooling velocity of the order $10^{-3} \dots 10^{-2}$ K/s, while for metallic glasses we have $q_c \approx 10^3 \dots 10^5$ K/s [2, 3]. The main emphasis in the proposed approach is on the common features of the transition to a non-crystalline state, namely, the study of the effect of non-equilibrium on formation of heterogeneous structures with $q \geq q_c$. For this purpose,

considered was the given speed $\tilde{q} = \frac{(q - q_c)}{q_c}$, which does not depend on the type of chemical bond. The processes of transition in the NCM for chalcogenide, oxide, metallic, and organic glass have the same features as the synergistic approach. Investigating the common nature, namely, the presence of processes of self-organization and formation of self-organized structures during the transition to NCS for different non-crystalline systems, it is possible at a later stage to consider the manifestation of the features for each of the above systems.

In the framework of this approach, correlation between the changes in force constants and fluctuations of the near, middle orders of non-crystalline materials is also determined. The most convenient model system for checking the processes of self-organization in the NCS is glass based As–S(Se). In the modern topological-cluster concept of the lattice structure, the connectivity of the matrix is inextricably related to its dynamic stability (quantitative measure of the dynamic stability of the glasses in the topological-cluster mechanistic model that includes elastic modules, which through the mean coordinate number reflect the dependence of the dynamic stability both on the structure and warehouse) [5]. For the

limit case of Ioffe–Regel, the length of the free path of phonons $l(k)$ with a wave vector $k = 2\pi/\lambda$ satisfies the ratio $l_{IR} \cdot k_{IR} = 1$ [1, 23], and the value opposite to it

$$\frac{1}{l} = 8 \frac{\Delta \bar{S}_{f,g}^2}{S_{f,g}^2} \cdot L_c^2 k^4. \quad (20)$$

Here, $\Delta \bar{S}_{f,g}^2$ is the mean-square fluctuations of the elastic modulus, L_c is the average spatial correlation area of fluctuations. For $k \geq k_{IR}$, where the ratio is executed $l_{IR} \cdot k_{IR} = 1$, and taking into account that the frequency of the boson peak ν_{BP} neutron scattering $2\pi\nu_{BP} = S_{f,g} \cdot k_{IR}$, for L_c get the ratio

$$L_c = S \frac{S_{f,g}}{\nu_{BP}}, \quad (21)$$

where $S = (\Delta \bar{S}_{f,g}^2)^{1/3}$. For the non-crystalline solids of As–S(Se) system $\nu_{BP} = 10 \dots 60$ cm $^{-1}$, $S \approx 0.7 \dots 0.8$, get it

$$L_c \approx 10 \dots 50 \text{ \AA}. \quad (22)$$

As you can see, the value L_c coincides with the nanosize of the middle order of NCS and indicates correlation of elastic properties and structure on the nanospatial scales [15]. For the speed of acoustic waves in NCS, the following empirical relation is obtained

$$\ln \left(\frac{S_f}{\rho} \right) = -0.0145 \cdot M_a + 11.989, \quad (23)$$

where M_a is the average atomic mass. For the NCS materials $M_a \approx 77 \dots 78$ atomic mass units and according to relation (9) at room temperature [15], one can get $f = 10^5$ dyn/cm, $S_f = 2.5 \cdot 10^5$ cm/s.

We analyze empirical relations for the temperature of softening of non-crystalline materials in terms of the considered synergetic model. In the theory of free volume between the softening temperature T_g , fraction of free volume σ_g and the energy generated by the interaction E_k , the relationship is established [2, 24]:

$$T_g = E_k / \sigma_g. \quad (24)$$

In particular, for inorganic glasses $\sigma_g = 0.037 \pm 0.002$. According to Figs. 2 and 4, taking into account the relation of a free volume with a continuum disordering at the level of the near-order $\sigma_g = \exp(1 + Q^*(1 + 2\zeta^*))$, for glasses As–S(Se) are $Q^* = 0.15 \dots 0.2$, $\zeta^* = 0.5 \dots 0.7$ [25, 26]. We get the value $\sigma_g = 0.035 \dots 0.04$, which agrees with empirically obtained in the theory of free volume.

The following example relates to an experimentally observed correlation between the softening temperature

and the melting point of a substance known as the rule of Kautzman [23, 26]:

$$T_g = (0.7 \pm 0.1) \cdot T_m. \quad (25)$$

As can be seen from Fig. 2, the temperature of transition to the non-crystalline state is given, and the melting factor satisfies the ratio: $\tau_c \approx (2/3) \cdot \tau_m$, which is consistent with the rule of Kautzman. According to conducted research (Eqs. (9) to (11), Figs. 2 to 4), the glass transition temperature T_g with an increase in the cooling velocity shifts to a region of lower temperatures that correlates with the Ritland–Bartenev ratio [25, 27]:

$$\ln(q) = -\frac{\Delta H}{R \cdot T_g} + C, \quad (26)$$

where ΔH is the change of enthalpy at transition, R – universal gas constant. The dependence of flow of negative entropy $dS_c(\tilde{q})$ is ascertained in (8), (15) from the surrounding environment and the corresponding entropy changes inside the system, which correspond to the minimum energy dissipation, makes it possible to disclose also the content of the Adam–Gibbs relation to change the configuration entropy [2, 24]:

$$\Delta S_c \approx \left(\frac{T - T_g}{T_g} \right)^\beta, \quad \beta = 0.41. \quad (27)$$

6. Conclusions

The model ideas on formation of self-organized structures in non-crystalline semiconducting solids as a method of the system self-organization, carried out in accordance with the technological conditions of obtaining, have been developed. It has been established that the value of external control parameter – the cooling velocity – is higher than the threshold in the non-crystalline system spontaneously generated in its own scale of ordering L_c ; the lifetime and period of heterogeneity of self-organized structures depend on the cooling velocity. In particular, for non-crystalline semiconductors of the system As–S(Se), the characteristic values of the magnitude ordering are $L_c \approx 10 \dots 10^2 \text{ \AA}$ and correlate with the nanosized of middle order. The three-dimensional bifurcation diagram in the coordinates of the order parameter, temperature, and the external control parameter – the cooling velocity – has been constructed, which takes into account the thermodynamic and kinetic aspects of the transition to a non-crystalline state. The existence of a triple point is shown, in which the three states are coinciding at a critical temperature and the limiting cooling velocity: crystalline, liquid, and non-crystalline. The nature of the bifurcation process of transition to a non-crystalline state has been defined. The comparison of the obtained theoretical conclusions with empirical correlations and experimental data for non-crystalline semiconductor materials of the system As–S(Se) is carried out.

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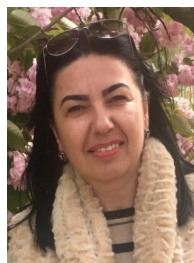
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