
MODELING OF MICROSTRUCTURAL CHANGES IN IRRADIATED SYSTEMS USING THE PHASE FIELD CRYSTAL METHOD

D.O. KHARCHENKO, V.O. KHARCHENKO, S.V. KOKHAN, I.O. LYSENKO

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Institute of Applied Physics, Nat. Acad. of Sci. of Ukraine
(58, Petropavlivska Str., Sumy 40030, Ukraine; e-mail: dikh@ipfcentr.sumy.ua)

Microstructural changes in systems subjected to the ballistic flux action have been studied. The formation of a structure disorder under irradiation has been described using the phase field crystal method. It is found that, owing to a competition between the regular and stochastic components of the ballistic flux, spatial patterns with smeared atomic densities can be formed. The dynamics of defects during the recrystallization in such systems has been studied, and the dependence of the variation in the number of defects on the statistical properties of a ballistic flux has been analyzed. The spatial patterns formed under the action of such flux during the recrystallization are found to be stationary and resistant to low-intensity thermal fluctuations.

1. Introduction

The study of a microstructure of crystalline materials, conditions under which it transforms, and the character of transformations is a challenging problem today not only from the viewpoint of theoretical physics, but also solid state physics and materials technology in general [1]. In recent years, the solution of this problem has become more and more important, because it is associated with the determination of the resistance of constructional materials used in various domains of human activity, in particular, in radiation equipment [2]. The evolution of such systems is governed by thermodynamic forces, mechanical loads, or radiation influence. The mechanical instability of crystalline systems results in the emergence of defects (point-like, linear, planar, and bulk ones), which are capable of strongly affecting the behavior of such systems under various conditions of their usage. Therefore, the understanding and the study of defect structure formation processes and defect dynam-

ics have been invoking a steady scientific interest within the last several decades.

In recent years, it was found that the adequate description of microstructural transformations can be reached by examining the behavior of such systems self-consistently at various hierarchical levels of the space-time scale ranging from quantum-mechanical to macroscopic ones [3]. A separate application of physical-theoretic methods at a definite hierarchical level of such a multiscale scheme does not allow a complete picture of the self-organization in a crystalline or defect structure to be constructed. For instance, *ab initio* methods allow the behavior of a system to be described at lengths of the order of 10^{-9} m and time intervals of about 10^{-14} s. The dynamics of atoms and point defects analyzed using the molecular dynamics methods is confined to intervals of 10^{-9} – 10^{-8} m in space and 10^{-13} – 10^{-8} s in time. It is worth noting that the number of atoms that can be traced while simulating such processes numerically is limited to a finite value; namely, the efficiency of *ab initio* approaches is limited by a consideration of 10^6 and molecular dynamics one of 10^9 atoms. The application of analytical approaches together with numerical techniques (Monte-Carlo kinetic simulation) in microstructural researches is used successfully enough at diffusion scales, where the examined system can be considered in the thermodynamic limit under certain boundary conditions. Among the most widespread approaches of this type, the phase field method, which is based on the Ginzburg–Landau theory, is distinguished [4].

However, among the mentioned approaches, we may address the so-called hybrid approaches and methods, which cover several hierarchical levels. The most popu-

lar and most used of them for the research of microstructures in materials is the phase field crystal method, which allows the crystalline systems of various symmetries to be described in the framework of a continuous field for the atomic density. The basis of the method was borrowed from hydrodynamics, where it was used for the description of the formation of Rayleigh–Bénard cells [5]. The physical content of its application to crystalline systems was substantiated in the theory of solidification [6], which was developed in the framework of the Ginzburg–Landau theory in works by Elder, Grant, and others [7]. In the framework of this approach, the crystalline phase is characterized by a periodically distributed field of atomic density $\rho(\mathbf{r})$, which corresponds to the minimum of the free energy functional $\mathcal{F}[\rho(\mathbf{r})]$. Its advantage over the standard phase field theory consists in the capability of a long-term modeling of the material evolution on the microscopic spatial scale. This method is also preferable as compared with the methods of molecular dynamics due to the exclusion of fast degrees of freedom, which allows the dynamics of a system to be studied within mesoscopic time intervals. This technique works as a tool for the time coarsening of the molecular dynamics τ (the averaging over phonons) [8]. In other words, instead of atomic positions, the corresponding atomic densities are considered as the probabilities for every i -th atom to fill the phase volume, i.e. $\rho(\mathbf{r}, \tau) = \tau^{-1} \int_0^\tau dt \rho_m(t)$, where $\rho_m(\mathbf{r}, t) = \sum_i^N \delta(\mathbf{r} - \mathbf{r}_i(t))$. Moreover, this approach allows one to simulate elastic and plastic deformations in crystals, liquid–solid phase transitions [9], defect diffusion [10], microstructural transformations [11], phase stratification, epitaxial growth, dislocation dynamics [12], and structural transitions [13, 14].

It is evident that the application of this method to studying the microstructural changes in irradiated substances and the behavior of defects at the recrystallization in relevant systems looks rather efficient. Since the combination of such an approach with the results of molecular dynamics is good, it becomes possible to detect the defect redistribution at the recrystallization, to study the motion of dislocations and grain boundaries, as well as the behavior of microcracks. In this case, it is necessary to introduce the corresponding forces and fluxes into consideration, which induce the formation of a structural disorder under irradiation. Taking advantage of the approaches developed in works [15–17], the influence of radiation inserting a structural disorder can be adequately described by introducing a ballistic (athermic) flux with atomic mixing into consideration. This flux stimulates an additional (ballistic) diffusion of atoms with stochastic character [18]. It is well known

that, in nonlinear distributed systems, the nonequilibrium fluctuations are capable of invoking a qualitative reorganization in the system, which is impossible under equilibrium conditions [19–21], e.g., phase transitions [22], phase separation [23], and structurization both in the bulk [24] and on the surface [25, 26]. Therefore, the issue concerning the influence of statistical properties of a ballistic flux on the microstructural transformations in crystalline systems seems to be important. In this case, the description of the formation of defects at irradiation and their annealing becomes possible [27–29].

Hence, this work is aimed at studying the character of microstructural transformations in irradiated crystalline systems with regard for a ballistic flux with stochastic properties (noise). To achieve this purpose, we applied the phase field crystal formalism. We will develop the general approach for the case of two-dimensional systems, which can be extended onto three-dimensional systems in the future. We will demonstrate that, owing to the stochastic influence, the metastable, but persistent structures with a symmetry different from that in the initial crystal can be realized in the system. We will study the processes of atomic density redistribution under the action of an athermic flux and elucidate the dynamics of defects at the recrystallization in the irradiated system.

The work structure is as follows. In the next section, the basic model of crystalline system is proposed, and the ballistic flux is introduced. In Section 3, the character of microstructure changes at irradiation and recrystallization is studied with the use of numerical simulation methods. The results obtained are discussed in Section 4. The last section contains conclusions.

2. Model

In the framework of the standard phase field crystal formalism, a periodic system (a crystal) and probable structural transitions in it are described as changes in the properties of the atomic density field $\rho(\mathbf{r}, t)$. Let us consider a one-component system with the property $\int d\mathbf{r} \rho(\mathbf{r}, t) = \rho_0 = \text{const}$, for which a variation of the free energy $\Delta\mathcal{F} = \mathcal{F}[\rho] - \mathcal{F}[\rho_0]$ looks like [12]

$$\frac{\Delta\mathcal{F}}{T} = \int d\mathbf{r} \{ \rho(\mathbf{r}) \ln[\rho(\mathbf{r})/\rho_0] - \Delta\rho(\mathbf{r}) \} - \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \Delta\rho(\mathbf{r}_1) c^{(2)}(\mathbf{r}_1, \mathbf{r}_2, \rho_0) \Delta\rho(\mathbf{r}_2),$$

where $\Delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \rho_0$, $c^{(2)}(\mathbf{r}_1, \mathbf{r}_2, \rho_0)$ is the two-point correlation function, the first term describes the

free system, and the second one characterizes the interaction. This expression is valid only if the variation $\Delta\rho(\mathbf{r})$ is small. However, the error of such an approximation amounts to a few percent, when the solidification processes are described. Therefore, under definite weak conditions, the formula above can be regarded as satisfactory [12].

The general formalism of the phase field crystal theory is based on the following two basic assumptions. Provided that $\Delta\rho(\mathbf{r})$ varies weakly when $c^{(2)}$ changes, the expansion in a series in the squared wavenumber gives rise to the expression $\rho_0 c^{(2)}(q) \simeq C_0 + C_2 q^2 + C_4 q^4$. The constants $C_0 < 0$, $C_2 > 0$, and $C_4 < 0$ determine the properties of a specific crystalline system (material); namely, these are the isothermal compressibility of the liquid phase (the dimensionless compression modulus of liquid state), $\sim 1 - \rho_0 C_0$, the compression modulus in the crystal phase, $\sim \rho_0 C_2^2 / 4 |C_4|$, and the lattice constant, $a_0 \sim \sqrt{|C_4| / C_2}$.¹ The expansion of the noninteracting part in a series in a vicinity of ρ_0 allows the free energy functional for the dimensionless atomic density field $x(\mathbf{r}) \propto \Delta\rho(\mathbf{r}) / \rho_0$ to be expressed in the form [14]

$$\mathcal{F} = \int d\mathbf{r} \left(f(x) + \frac{1}{2} x \mathcal{L}(\nabla^2) x \right), \quad (1)$$

where the free energy density $f(x)$ and the operator of spatial interaction $\mathcal{L}(\nabla^2)$ are given by the equations

$$f(x) = \frac{\alpha(T - T_m)}{2} x^2 + \frac{u}{4} x^4, \quad \mathcal{L}(\nabla^2) = \beta(q_0^2 + \nabla^2)^2, \quad (2)$$

which are expressed in terms of the material constants α , u , and β ; T_m is the melting temperature; and q_0 is the wavenumber that determines the lattice parameter. A relation between the parameters of the theory and the microscopic parameters of a specific crystalline system can be found according to the procedure described, e.g., in work [14].

Since the atomic density field is a conserved quantity, its Langevin dynamics is given by the equation

$$\partial_t x = M \nabla^2 \frac{\delta \mathcal{F}}{\delta x} + \xi, \quad (3)$$

where $M = \text{const}$ is the atomic mobility, and the white noise ξ is characterized by standard properties $\langle \xi(\mathbf{r}, t) \rangle = 0$ and $\langle \xi(\mathbf{r}, t) \xi(\mathbf{r}', t') \rangle = 2MT \nabla^2 \delta(\mathbf{r} - \mathbf{r}') \delta(t - t')$.

¹ The lattice parameter $a_0 = 2\pi/q_0$ is determined by the wavenumber $q_0 = \sqrt{3C_2/8|C_4|}$ in the two-dimensional case and by the wavenumber $q_0 = \sqrt{C_2/|C_4|}$ in the three-dimensional one [12].

For the further consideration, it is expedient to renormalize some quantities,

$$\mathbf{r}' = \mathbf{r} q_0, \quad x' = x \sqrt{u/T_m \beta q_0^4}, \quad \varepsilon' = \alpha \Delta T / T_m \beta q_0^4,$$

$$t' = M \beta q_0^6 t, \quad \mathcal{F}_0 = \beta^2 q_0^{8-d} T_m / u, \quad \mathcal{F}' = \mathcal{F} / \mathcal{F}_0, \quad (4)$$

introduce the control parameter $\varepsilon = \theta - 1$ into consideration, and renormalize the fluctuation source,

$$\langle \xi(\mathbf{r}, t) \rangle = 0,$$

$$\langle \xi(\mathbf{r}, t) \xi(\mathbf{r}', t') \rangle = \frac{u \theta q_0^{d-4}}{\beta^2} \nabla^2 \delta(\mathbf{r} - \mathbf{r}') \delta(t - t'). \quad (5)$$

In what follows, the primes will be omitted for convenience. It should be noted that, provided definite conditions in the system (a selected value of the density, x_0), the realization of structures of the hexagonal type (a periodic distribution of the atomic density) and the so-called stripes (linear structures) becomes possible. Anyway, the emergence of spatial structures is probable only provided that $x_0 \leq \sqrt{1 - \theta}$, i.e. if the free energy density is bimodal. Otherwise, the system is uniform irrespective of the selected density value. In the case of a two-dimensional system for $\mathcal{L} = (1 + \nabla^2)^2$, the general solution of the equation of state can be expressed in the form

$$x(\mathbf{r}, t) = x_0 + s(t)(e^{i\mathbf{k}_1 \mathbf{r}} + \text{c.c.}) + h(t)(e^{i\mathbf{k}_2 \mathbf{r}} + e^{i\mathbf{k}_3 \mathbf{r}} + \text{c.c.}),$$

where c.c. means complex conjugation; $s(t)$ and $h(t)$ are amplitudes; and the wave vectors are as follows:

$$\mathbf{k}_1 = \left(-\frac{\sqrt{3}}{2}, -\frac{1}{2} \right); \quad \mathbf{k}_2 = (0, 1), \quad \mathbf{k}_3 = \left(\frac{\sqrt{3}}{2}, -\frac{1}{2} \right).$$

Therefore, in the case $s = h$, we have the hexagonal crystalline phase (a periodically distributed atomic density). This means that every atom moves in a vicinity of its equilibrium position, all atoms move in a spherically symmetric region in vicinities of their positions arranged periodically with the lattice period $a = 2\pi/q_0$, and the frequency of stay at every point in a vicinity of the equilibrium position \mathbf{r}_i is determined by the quantity $x_0(\mathbf{r}_i)$. If $h = 0$, linear structures are realized. This means that, although the atomic density distribution in the stationary case has a periodic structure corresponding to atomic planes, it is smeared in parallel to those planes, because atoms can move along them. In the range of uniform

states, $s = h = 0$, the atomic density is smeared over the whole system, so that the latter is actually in the liquid state. There may arise regions, in which the crystalline (hexagonal) phase and uniform states coexist; it is also true for the coexistence region of hexagonal and linear structures. This problem was studied earlier (see, e.g., work [30], where the critical values for the realization of the described structures in one- and two-dimensional cases were found). Using the methods of numerical simulation, the features in the periodic structure formation were studied for the atomic density distribution in three-dimensional systems, and a possibility for the fcc, bcc, and hcp structures (in the two-dimensional case, they correspond to the domain of hexagonal phase existence) to emerge in three-dimensional systems was established [31, 32]. Earlier, it was shown [7] that the elastic properties of the hexagonal phase in the two-dimensional case are described by the elastic constants $C_{12} = C_{44} = C_{11}/3$, where $C_{12} = [(3x_0 + \sqrt{-15\varepsilon - 36x_0^2})q_0^2]/75$ and $C_{11} = C_{12} + 2C_{44}$, with Poisson's ratio $\nu = 1/3$, the shear modulus $\mu = C_{44}$, and the Young modulus $Y_2 = 8C_{12}/3$.

The irradiation influence will be taken into account by introducing the athermic mixing flux in the atomic system [18],

$$\mathbf{J}_e = -(D_e + \zeta(\mathbf{r}, t))\nabla x, \quad D_e = \phi\langle R \rangle^2\sigma_r, \quad (6)$$

which has regular and stochastic components. The regular part characterizes the radiation-induced diffusion. It depends on the coefficient of ballistic diffusion D_e expressed in terms of the irradiation flux ϕ , the average hop distance $\langle R \rangle$ for a knocked-out atom, and the scattering cross-section σ_r . In turn, the quantities σ_r and $\langle R \rangle$ depend on the energy of bombarding particles. The stochastic component describes the formation of a structural disorder and has Gaussian properties. Since a stochastic mixing in a structured medium (a crystal) is considered, it is evident that the random component should be correlated in space. Let its properties be selected as follows:

$$\langle \zeta(\mathbf{r}, t) \rangle = 0,$$

$$\langle \zeta(\mathbf{r}, t)\zeta(\mathbf{r}', t') \rangle = \frac{2D_e\sigma^2}{(\sqrt{2\pi}r_c)^d} e^{-(\mathbf{r}-\mathbf{r}')^2/2r_c^2} \delta(t-t'). \quad (7)$$

The presence of D_e in the expression for the correlator testifies that the noise ζ arises only if the irradiation flux does exist. The noise intensity $\sigma^2 = \langle (\delta R)^2 \rangle / \langle R \rangle^2$ is connected with the length dispersion for jumps made by knocked-out atoms, and r_c is the radius of spatial

correlations. Such a construction of the athermic mixing flux allows one to consider cases that are not reduced to the conventional diffusion described by the Laplacian in the evolution equation, but also lead to a generalized stochastic character of motion with a given dispersion of jump lengths, $\langle (\delta R)^2 \rangle$. Therefore, in what follows, it is expedient to consider the quantities D_e and σ^2 as two independent parameters of the theory [18]. Hence, the total evolution equation for the atomic density field reads

$$\partial_t x = \nabla^2 \frac{\delta \mathcal{F}}{\delta x} + \xi(\mathbf{r}, t) + \nabla \cdot (D_e + \zeta(\mathbf{r}, t))\nabla x. \quad (8)$$

The features in the formation of a periodic distribution of the the atomic density in a system with the athermic mixing flux described by Eq. (8) were analyzed in work [33] for various initial values of atomic density. The behavior of a nonequilibrium system, for which the times of the perturbation propagation through the athermic and usual diffusion fluxes are different, was considered in work [34]. It was found that, irrespective of the initial value of $x(\mathbf{r}, t = 0)$, the action of a correlated stochastic source $\zeta(\mathbf{r}, t)$ can transform the system into a state with linear structures. In other words, the irradiation-induced emergence of a structural disorder in a correlated medium gives rise to a change of the crystal microstructure, the appearance of ordered phases separated by disordered ones, the smearing of the atomic density over atomic planes, and the density distribution homogenization, i.e. the crystal melting. However, the nature of transitions from hexagonal to linear structures under the action of an external stochastic source has not been studied.

Despite that the processes of ordered configuration formation were studied earlier, the microstructural changes and the formation of defects under the athermic mixing were not analyzed. Therefore, this work is aimed at elucidating the behavior of the formation of defects in a crystalline system subjected to the action of an athermic mixing flux. The main properties of the defect structure formation are studied in the framework of the geometrical approach, and the distortions in the perfect hexagonal structure owing to the formation of dislocations are determined.

3. Features of microstructural changes

3.1. Linearized model. Structure factor

Let us consider firstly the system in the framework of a linearized model in a vicinity of the examined density x_0 .

Since x is a conserved quantity, the stability analysis is carried out for the spherically averaged structure factor $S(k, t)$, which is the Fourier transform of the two-point correlation function $\langle \delta x(\mathbf{r}, t) \delta x(\mathbf{r}', t) \rangle$, where $\delta x(\mathbf{r}, t) = x(\mathbf{r}, t) - x_0$. According to the Novikov theorem [35], the dynamic equation for $S(k, t)$ looks like

$$\frac{dS(k, t)}{dt} = -2k^2\omega(k)S(k, t) + 2\theta k^2 + \frac{2k^2 D_e \sigma^2}{(2\pi)^d} \int d\mathbf{q} C(|\mathbf{k} - \mathbf{q}|) S(\mathbf{q}, t), \quad (9)$$

where $C(|\mathbf{k} - \mathbf{q}|)$ is the Fourier transform of the external noise correlation function. In this case, the dispersion law reads

$$\omega(k) = \tilde{\varepsilon} + D_e + (1 - k^2)^2 - D_e \sigma^2 C(0) k^2 + D_e \sigma^2 [\nabla^2 C(|r|)]_{r=0}, \quad (10)$$

where $\tilde{\varepsilon} \equiv \varepsilon + 3x_0^2$ and $[\nabla^2 C(|r|)]_{r=0} < 0$, because the noise correlator has a maximum at the point $r = 0$. From the relation obtained, it follows that the external flux renormalizes the control parameter so that the behavior of the system is now governed by its effective value

$$\varepsilon_{\text{ef}} = \tilde{\varepsilon} + D_e + D_e \sigma^2 [\nabla^2 C(|r|)]_{r=0}. \quad (11)$$

It is evident that if $\varepsilon_{\text{eff}} < 0$, the perturbations of harmonics in a vicinity of $k_0 = 1$ grow, which results in the formation of periodic structures. Whence it follows that the regular component D_e of the athermic flux brings about an increase of the effective temperature. If the particles in the irradiation flux have an energy (momentum) spread, i.e. $\sigma^2 \neq 0$, then, taking into account that $[\nabla^2 C(|r|)]_{r=0} < 0$, the stochastic component of the flux \mathbf{J}_e violates the stability by reducing the value of effective control parameter. Hence, the regular and stochastic components of the irradiation flux \mathbf{J}_e influence oppositely the dynamics of the system, which agrees with the results obtained in the framework of the mean-field theory for deterministic systems [15] and in the analysis of the behavior of systems with a stochastic irradiation flux [18]. A detailed analysis of the influence exerted by the stochastic component of the athermic mixing flux on the stability of uniform states was carried out in detail in works [33, 34, 36–38]. It was found that, contrary to intuitive reasonings concerning the noise influence, the action of a spatially correlated stochastic source in systems with conserved dynamics gives rise to a spatial ordering [19, 39–41].

From the dispersion law, we can determine the critical values of wave numbers, $k \in (k_c^{(-)}, k_c^{(+)})$, that confine the domain of existence for the unstable modes,

$$(k_c^{(\pm)})^2 = 1 + \frac{1}{2} \left(D_e \sigma^2 C(0) \pm \left\{ D_e \sigma^2 C(0) (4 + D_e \sigma^2 C(0)) - 4(\tilde{\varepsilon} + D_e - D_e \sigma^2 [\nabla^2 C(|r|)]_{r=0}) \right\}^{1/2} \right). \quad (12)$$

For such values of wave numbers, the gain factor $R(k) = -k^2\omega(k)$ equals zero. The maximum of the function $R(k)$ is attained at $k = k_m$, where

$$(k_m)^2 = \frac{2}{3} + \frac{1}{3} \left(D_e \sigma^2 C(0) \pm \left\{ 1 + D_e \sigma^2 C(0) (4 + D_e \sigma^2 C(0)) - 3(\tilde{\varepsilon} + D_e - D_e \sigma^2 [\nabla^2 C(|r|)]_{r=0}) \right\}^{1/2} \right). \quad (13)$$

At high temperatures and a fixed D_e -value, the critical value of σ^2 increases, whereas the growth of D_e stimulates the ordering at a lower noise intensity σ^2 .

The dynamics of the structure factor obtained as a solution of Eq. (9) is depicted in Fig. 1. The figure demonstrates that, as the time grows, the position of the main $S(k, t)$ peak is shifted to the wave number $k = k_0$, which corresponds to the period of emerging structures. The peak height increases at that, which testifies that the ordering in the system becomes stronger.

3.2. Modeling of microstructural transformations

Let us analyze a variation of the behavior of the system, when the grown crystal is first subjected to the irradiation within a definite time interval so that the defects emerge in its crystalline structure and, afterward, to the annealing. Such a procedure was simulated numerically. For this purpose, we found a numerical solution for the Langevin equation (8) on a two-dimensional square mesh of the dimension $L = N\ell$, where $N = 256$ is the number of nodes and $\ell = 1$, with periodic boundary conditions.

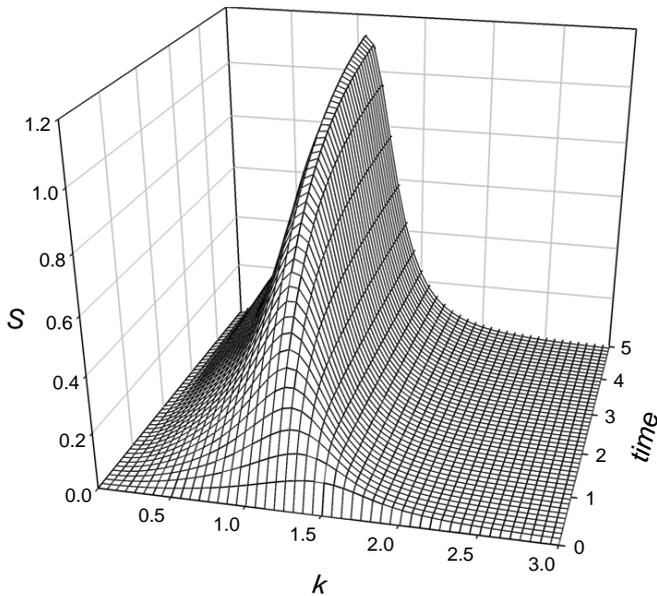


Fig. 1. Dynamics of the structure factor averaged over the sphere in a vicinity of $x_0 = 0.3$ at $D_e = 0.8$, $\theta = 0.7$, $\sigma^2 = 1.0$, and $r_c = 1$

At the stage of crystal growth from the liquid phase, the initial conditions were selected as follows: $\langle x(\mathbf{r}, t) \rangle = 0.3$ and $\langle (\delta x)^2 \rangle = 0.1$. All results were obtained at $\theta = 0.7$ and $r_c = 0.65$.

A typical scenario of the formation of a crystal from the liquid phase is shown in Fig. 2. Crystallites grow from the crystal phase nuclei distributed over the whole specimen, until they match one another. After the whole system becomes filled with the hexagonal phase, the subsequent evolution continues through the motion of grain boundaries. When the basic structure is formed, the “atoms” (dark circles) become redistributed in such a way that the emerging configuration should have the smallest number of defects by tending to the minimum energy of the whole object. A characteristic dimensionless time of crystal growth was $t = 2 \times 10^4$, which corresponded to a transition to the stationary mode and a reconstruction of the atomic configuration accompanied by a reduction of the defect number. In what follows, this object will be subjected to the irradiation with various D_e and σ^2 . The main task at the next stage will be the study of the defect number dynamics and the features of the microstructure reorganization at irradiation and recrystallization.

First, let us consider the basic scenarios of microstructural changes in the initial crystalline specimen at its irradiation. The patterns shown in the first column of Fig. 3, *a* illustrate the influence of the regular component of the athermal mixing flux ($\sigma^2 = 0$). One can

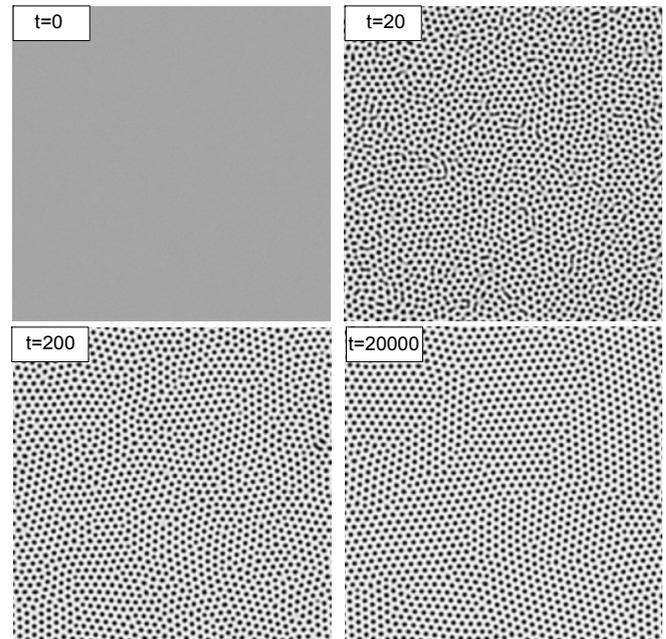


Fig. 2. Patterns of the evolution of the system at the stage of crystal growth at $\theta = 0.7$

see that the defects segregated at grain boundaries melt as the time increases. Accordingly, the most resistant structures, which correspond to a perfect configuration with hexagonal symmetry, survive. At the final stage and for small D_e -values, there remain crystallites with a perfect structure imbedded into the disordered phase, in which the atomic density is smeared over all atomic positions. This means that, in our model, the passage of continuous cascades stimulates the melting in those regions, where the energy is higher than that contained in ideal crystalline ones. The dimensionless time of irradiation was $t = 10^3$, which corresponded to the realization of a stationary structure. In effect, this scenario characterizes, in general, the evolution of extra (radiation-induced) diffusion processes, when the defects become mobile. At the same time, the structures with a considerable number of defects are unstable with respect to such perturbations. From the definition of effective control parameter (11), it follows that the influence of the regular component of the athermal mixing flux elevates the effective temperature and shifts the system into the liquid phase region or into the region, where the crystalline and liquid phases coexist. For large D_e , the effective temperature becomes so high that the initial crystalline system already falls within the region of the liquid (melt) phase.

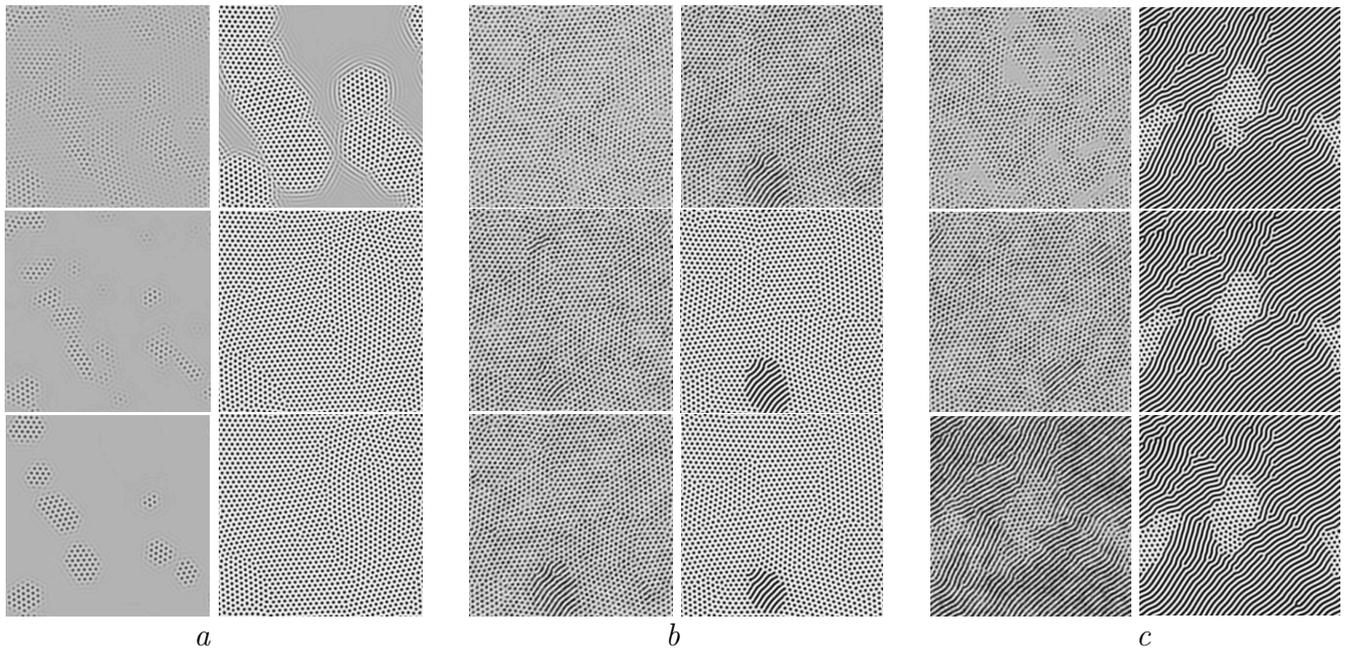


Fig. 3. Patterns of the evolution of the system at the irradiation and recrystallization stages. The first columns in panels *a* to *c* correspond to the irradiation process with the parameters $D_e = 0.35$, $\sigma^2 = 0.0$ (*a*); $D_e = 0.475$, $\sigma^2 = 0.3$ (*b*); and $D_e = 0.55$, $\sigma^2 = 0.3$ (*c*). The second columns illustrate the evolution of the system at the recrystallization in the corresponding irradiated structures

Now, let our system be subjected to the recrystallization (see column 2 in Fig. 3,*a*). Provided that the last configuration is selected as the initial one at this stage and putting $D_e = 0$, the corresponding crystallization processes will proceed from available crystallites. Here, the wave of atomic perturbations will extend uniformly along all possible directions in such a manner that atoms, by arranging themselves to the main crystallite, will promote the formation of a perfect grain structure. The number of initial crystallites at the recrystallization can vary depending on the D_e -value. Therefore, the total number of defects that survive at the final stage of this process can also undergo changes.

More interesting is the stochastic case where the irradiation occurs in the presence of athermal flux fluctuations ($\sigma^2 \neq 0$). Here, depending on the ratio between the regular and stochastic components of this flux, the structures of two types are possible in the stationary regime. The regular and stochastic components of the flux \mathbf{J}_e compete for a modification of the effective temperature (see Eq. (11)). Therefore, for instance, if the intensity σ^2 is fixed, and the D_e -value is small, the external noise will counteract the melting of crystalline regions. In this case, the atomic density decreases locally, but the geometrical structure remains almost invariable. At elevated D_e -values (see column 1 in Fig. 3,*b*), the ac-

tion of noise in the melted regions in a vicinity of the grain boundaries stimulates the ordering with the formation of linear structures (stripes), in which the atomic density, although being distributed periodically in accordance with the arrangement of atomic planes, is smeared in those planes. In other words, atoms wander over atomic planes in the emerged structure. If the D_e -value increases further (see column 1 in Fig. 3,*c*), the crystalline system melts owing to the action of the regular component of the flux \mathbf{J}_e . Simultaneously, it gets structured and forms stripes due to the correlation effects of the stochastic source. Hence, such a character of the irradiation promotes the knocking-out of atoms from their positions and makes them wandering over atomic planes. On the other hand, if the external noise intensity is increased at a fixed D_e -value, the system turns out in the domain of existence for stationary structures of the linear type. Similar effects were observed at the Monte-Carlo atomic simulation, when crystallites imbedded into the melted regions coexisted with a configuration with the atomic density smeared over the atomic planes [42–44].

The stochastic and deterministic cases of the recrystallization in the irradiated system differ from each other. Really, in the former case, not only the crystallites with a lower symmetry, but also the structures with a higher symmetry must be rearranged to match genuine crys-

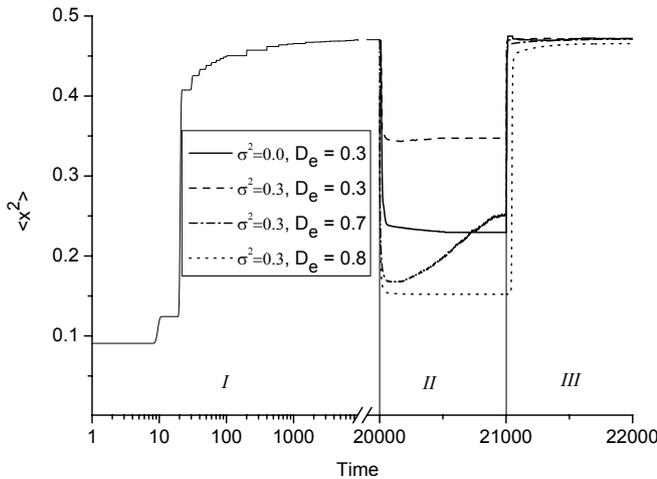


Fig. 4. Dynamics of the order parameter $\langle x^2 \rangle$ at various D_e and σ^2 . Stage I corresponds to the growth of the initial crystal, stage II to the irradiation stage, and stage III to the recrystallization stage

talline ones. This process is rather long. However, after its termination, every linear structure starts to detach its atoms one-by-one, which expands the region occupied by crystallites. The scenario of such a recrystallization is depicted in columns 2 of Figs. 3,*b* and *c*. In the case where the system is mainly in the hexagonal phase (column 2 in Fig. 3,*b*), a redistribution of the atomic density over the crystal configuration takes place firstly in order to reduce the defect number and to form a perfect crystalline structure. Then the detachment of atoms from linear structures occurs (local cooling of atoms wandering over the planes). In the case shown in column 2 of Fig. 3,*c*, the linear structures with defects have to be redistributed in such a way that they should occupy positions compatible with the atomic plane directions. After that, the formation of crystallites may take place depending on the ratio between the system fractions in the hexagonal and stripe phases.

To make a quantitative analysis of the ordering/disordering processes, let us trace the behavior of the second statistical moment $J(t) = N^{-2} \langle \sum_{\mathbf{r}} x_{\mathbf{r}}^2 \rangle$, which plays the role of order parameter in systems with conserved dynamics and which is known as the convective flux in the theory of structure formation [19]. Generally speaking, for the systems with conserved and non-conserved dynamics, it is known that the growth of this parameter in time testifies that the ordering processes run in the system. In Fig. 4, the dynamics of the order parameter at various stages is presented. Stage I corresponds to the crystal growing, stage II to irradiation under various conditions, and stage III to the recrystallization in the system. As one can see, if $\sigma^2 = 0$ (the

solid curve), the switch-on of the athermal flux results in a reduction of the order parameter, and if irradiation is switched off (stage III), the system quickly relaxes to the stationary value of order parameter, which was observed at the crystal growing. In the stochastic case (the dashed curve) and at a fixed D_e , the order parameter falls down to a stationary value that exceeds the value reached in the deterministic case. This fact testifies that the external fluctuations support the ordered state owing to their correlated actions. If the parameter D_e increases (the dash-dotted curve) and if the intensity σ^2 remains constant, the system melts at the initial stage of irradiation, whereas noise favors the ordering by raising the value of $\langle x^2 \rangle$ at late stages. At large D_e 's, the correlation properties of the external noise support the ordering in the system; nevertheless, the system becomes disordered in the sense that the crystal becomes reorganized into a structure of linear objects. In the course of crystallization, the restoration of a crystalline configuration in the irradiated system at large D_e 's proceeds in such a manner that the order parameter does not reach its stationary value corresponding to the grown crystal. Hence, the introduction of additional perturbations into the initial configuration can promote the emergence of spatial structures of other types at the recrystallization. This effect can evidently be associated with a correlated mixing of the system, when the processes of interaction induced by noise in the atomic system, the redistribution of defects, and the variation of their number begin to play a dominant role.

As follows from the simulation results, the character of ordering in the irradiated system substantially depends on the irradiation conditions. Accordingly, the type of defects and their number at the recrystallization can change. It should be noted that the $\langle x^2 \rangle$ -value, which is proportional to the area under the structure factor, is an integrated characteristic and cannot serve as an indicator of microstructural changes in the crystal. Therefore, we will study the geometry of obtained structures by calculating the number of defects, their evolution, and the characteristics of disordered configurations. In the framework of the formalism used below, we distinguish two types of defects, point-like defects (stacking faults) in a crystalline system with the hexagonal symmetry and linear defects (dislocations) in a system of linear structures.

In the case where the system recrystallizes into the hexagonal phase, let us determine the stacking faults following the algorithm developed for studying the two-dimensional systems, which were simulated with the use of molecular dynamics methods [45]. In the framework of

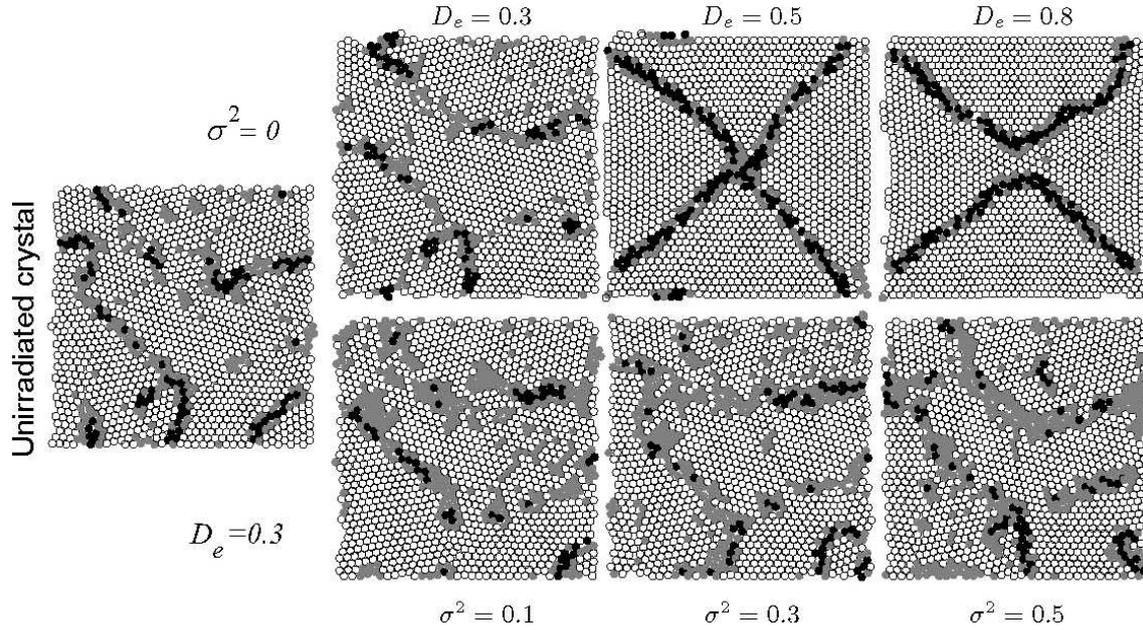


Fig. 5. Patterns illustrating the structure imperfection in the irradiated system at its recrystallization from the initial configuration shown to the left. The upper row corresponds to the irradiation at various D_e and a fixed intensity σ^2 ; the lower one to the irradiation at various σ^2 and a fixed D_e

this approach, real atoms, which the molecular dynamics deals with, are replaced by virtual “atoms” of the phase field crystal method. At the same time, the hexagonal symmetry is studied similarly. The major steps of this method are as follows. The local crystalline order can be described in terms of the orientation of hexagons, the vertices of which correspond to the maxima of the atomic density $x(\mathbf{r}, t)$. Then the orientation angle for the j -th atom, $\alpha_j \in [0, \pi/3]$, is determined from the relation $\Psi_j = \sum_{k \in nn(j)} \exp[6i\theta_{jk}] = |\Psi_j|e^{6i\alpha_j}$. Two atoms are neighbors, if $|\mathbf{r}_j - \mathbf{r}_k| < 1.25\nu$, where ν is the position of the first peak of the two-particle correlation function, and θ_i is the angle between the corresponding vector $\mathbf{r}_j - \mathbf{r}_k$ and the x -axis. The disorder degree for the j -th atom is determined by the formula

$$D_j = 2 \sum_{k \in nn(j)} [1 - \cos 6(\alpha_i - \alpha_k)].$$

The quantity D_j is usually plotted in color, which allows the imperfection of a crystal structure geometry to be estimated visually. In our case, we plotted it on the gray scale: white circles correspond to the perfect geometry of the hexagonal phase, and black ones mark the most defect structures, when the number of the nearest neighbors for the j -th atom substantially differs from six. The black circles form grain boundaries. A typi-

cal pattern that illustrates a local disorder after the recrystallization is shown in Fig. 5. Here, circles stand for atoms (points with the maximum atomic density), and their colors correspond to the value of local disorder parameter for every atom. The pattern for the initial crystal is depicted to the left. The indicated parameters inform about irradiation conditions. The upper row, which corresponds to the case $\sigma^2 = 0$ and various D_e -values, makes it evident that the more melted was the initial crystal at the final stage of recrystallization, and the larger grains are obtained, which agrees well with the results of recrystallization theory. In the stochastic irradiation case with $D_e = 0.3$, the growth of noise in a definite interval can stimulate the segregation of defects at grain boundaries.

This procedure was used to calculate the number of defects, the latter being interpreted as atoms participating in the formation of stacking faults such as vacancies, interstitial atoms, and dislocation cores. The dynamics of the relative defect number $N_{\text{def}}/N_{\text{atom}}$, where N_{atom} is the total number of atoms (peaks in the atomic density), calculated for the recrystallization in the irradiated system with $\sigma^2 = 0$ is plotted in Fig. 6,a. One can see that, as the time grows, the number of defects falls down to a certain stationary value. Such a scenario is typical, when the recrystallization after the passage of cascades is simulated with the use of molecular dynam-

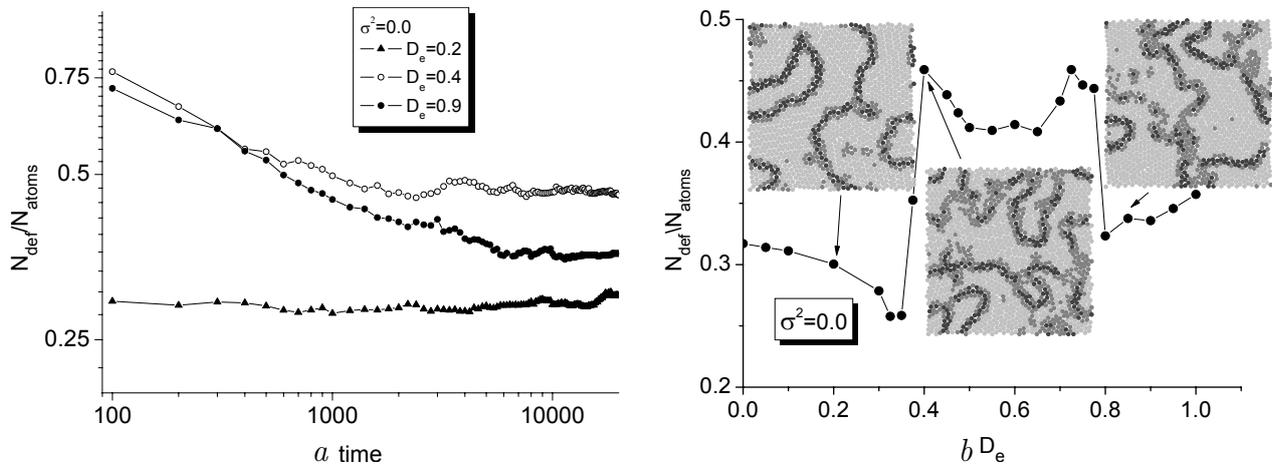


Fig. 6. Dynamics (a) and stationary dependences (b) of the relative defect number at $\sigma^2 = 0.0$ and various intensities of ballistic mixing

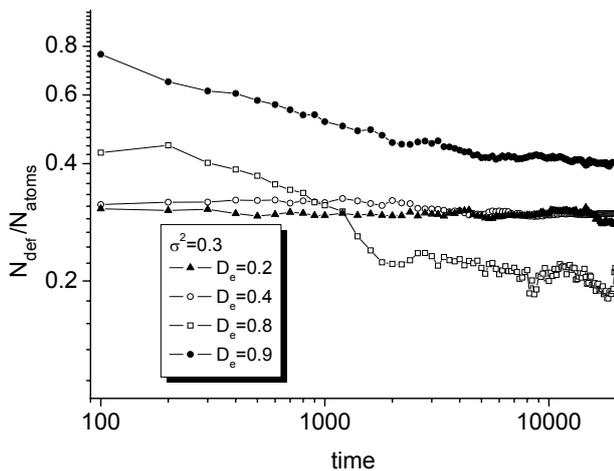


Fig. 7. Dynamics of the relative defect number at $\sigma^2 = 0.3$, $\theta = 0.7$, and various intensities of ballistic mixing

ics methods [46, 47]. From Fig. 6,a, one can see that the number of defects remains constant at small D_e -values, when the specimen is not changed practically under the weak action of radiation. However, when D_e increases, a considerable amount of defects (approximately 75% of the number of atoms) emerges. Their number falls down firstly following the power law $t^{-\delta}$ with $\delta \approx 0.2$, then – within diffusion time intervals – logarithmically slowly. In Fig. 6,b, the dependence of the number of defects that survived after the recrystallization (in the stationary case) on the intensity D_e is exhibited, and some patterns of the imperfect geometry in typical structures are illustrated. From this figure, one can see that, if the intensity D_e grows from the zero value, which is characteristic of the non-irradiated system, c number of defects

gradually diminishes. Since the growth of D_e leads to an elevation of the effective temperature, such a behavior of N_{def} means a reduction in the number of defects (grain coarsening) when the heated system recrystallizes. This is accompanied by a redistribution of atoms and a reduction of the crystal energy. At the characteristic values of ballistic mixing intensity, there are two peaks in the dependence $N_{\text{def}}(D_e)$. They actually correspond to the “phase” transition points for an equilibrium system, the effective temperature of which equals $\theta_{\text{eff}} = \theta + D_e$. The critical D_e -values lie along the curves in the equilibrium phase diagram $\theta_{\text{eff}}(x_0)$ that bound the domain of existence of the hexagonal phase. In such a sense, the stationary dependence $N_{\text{def}}(D_e)$ plays the role of effective geometrical susceptibility for the processes of structure formation in systems described by the phase field crystal theory.

In the case of irradiation and a stochastic source, the competition between the regular and stochastic components of the athermic flux results in that, if either D_e is small or D_e is large and σ^2 is small, the system transforms, after the recrystallization, into the state with the hexagonal phase. In this case, the proposed formalism for the determination of point defects can be applied. The corresponding time dependence of the defect number is depicted in Fig. 7, where the behavior of N_{def} is similar to that obtained in the deterministic case. Here, on the contrary, the number of defects does not diminish at analogous D_e -values, e.g., at $D_e = 0.4$. This fact is associated with the maintenance of the initial crystalline structure under the irradiation by the noise so that the number of defects practically is not changed in this case.

In the case where the noise intensity is comparable with the D_e -value or exceeds it, the system microstructure changes. Stripes (linear structures) rather than the hexagonal phase are realized. In this case, the indicated procedure for determination of defects cannot be applied, because the atomic density is smeared over the atomic planes. Defects, which can be researched in this case, include dislocations, disclinations, and grain boundaries. In our case, we did not observe grain boundaries, and disclinations comprised less than 1% of the total defect number. Therefore, in what follows, we concentrated our attention to studying the linear defects.

While studying the dislocations, let us take advantage of the approach developed for the analysis of defects in nematics [48]. Here, the nematic order parameter $Q_{\alpha\beta} = Q_0 [\hat{n}_\alpha \hat{n}_\beta - \frac{1}{2} \delta_{\alpha\beta}]$, where $\hat{n}(\mathbf{r}) = \frac{\nabla x(\mathbf{r})}{|\nabla x(\mathbf{r})|}$ is the aligning field (the director), is one of the ordering criteria. In particular, the quantity $\cos(2\theta)$, where $\hat{n} = (\cos(\theta), \sin(\theta))$, plays the role of order parameter for two-dimensional systems. This means that there exists a certain vector order parameter $\hat{\mathbf{B}}$ defined by the expressions $\hat{B}_x = \hat{n}_x^2 - \hat{n}_y^2$ and $\hat{B}_y = 2\hat{n}_x \hat{n}_y$. We will assume below that all defects are formed from $\pm \frac{1}{2}$ -disclinations in the aligning field \hat{n} , which transform into “vortices” of charge ± 1 in the field $\hat{\mathbf{B}}$. For the defect identification, let us define the cores of vortices by the formula $A = \sum_{\alpha,\beta} (\nabla_\alpha B_\beta)^2$. Within the defect region, the parameter $\hat{\mathbf{B}}$ changes drastically. Therefore, the location of a defect is determined from the condition that A exceeds a definite value. We can also express A in the form

$$A = \sum_{\alpha,\beta} (\nabla_\alpha n_\beta)^2 = (\nabla_\alpha \varphi)^2,$$

where $\varphi(\mathbf{r}, t) = 2\theta(\mathbf{r}, t)$ and $\theta(\mathbf{r}) = \arctan\left(\frac{\hat{n}_y(\mathbf{r})}{\hat{n}_x(\mathbf{r})}\right)$. The nematic order parameter $Q_{\alpha\beta}$ is completely determined by the angle $\varphi(\mathbf{r}) = 2\theta(\mathbf{r})$. Hence, knowing the derivative $\nabla\varphi(\mathbf{r})$ and calculating the indicator quantity $A(\mathbf{r}) = |\nabla\varphi(\mathbf{r})|^2$, we can reveal such defects as dislocations, disclinations, and grain boundaries.

The procedure is based on the fact that the field $\varphi(\mathbf{r})$ changes quickly in the defect (dislocation, disclination, or grain boundary) regions and slowly outside them. Therefore, defects or some part of the grain boundary are located at points, where $\varphi(\mathbf{r})$ varies more intensively. On the contrary, in the region beyond defects, $A(\mathbf{r}) \approx 0$. In a vicinity of the defect, this quantity grows drastically. The described algorithm helps us to find regions, where the director field changes substantially. Hence, the state of a system and the presence of grains and defects in it can be determined at an arbitrary moment.

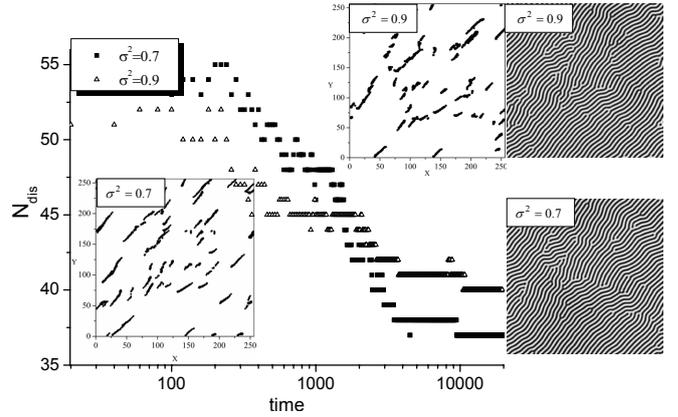


Fig. 8. Dynamics of the dislocation number at $D_e = 0.3$. The insets illustrate the trajectories of motion of dislocation cores calculated at $\sigma^2 = 0.7$ and $\sigma^2 = 0.9$, as well as typical patterns of stationary linear structures. The other parameters are $\theta = 0.7$ and $r_c = 1$

The application of the described formalism allowed us to estimate the number of dislocations and to determine their motion. In Fig. 8, the variation dynamics for the dislocation number N_{dis} , the trajectories of dislocation cores moving in the two-dimensional space, and typical stationary linear structures are exhibited. The behavior of the dislocation number parameter testifies that it slightly increases as the recrystallization begins, owing to the structure reorganization to the most optimum one possessing a lower elastic energy. Somewhat later, when the recrystallization terminates, the dislocations move and redistribute the accumulated elastic energy by annihilating with dislocations of the opposite charge. Within large time intervals, the dislocations slow down, and their number remains invariable. Hence, a system with the structure reorganized due to the action of irradiation may remain with a smaller number of defects, but its structure may not coincide with that in the initial non-irradiated crystal.

The presented procedure of defect detection allows one to obtain the stationary dependence of the defect number on the ballistic diffusion coefficient D_e in the stochastic case. The corresponding result is exposed in Fig. 9. It is evident from the figure that, in this case, similarly to what took place under the condition $\sigma^2 = 0$ (see Fig. 6,b), there are two critical values of intensity D_e . However, in contrast to the case of a deterministic system, no peaks can be detected now in the defect-number dependence, because the peaks correspond to the coexistence of stripes and the hexagonal phase. However, it is of importance that the phase of linear objects is realized in the range of critical D_e -values. Hence, the

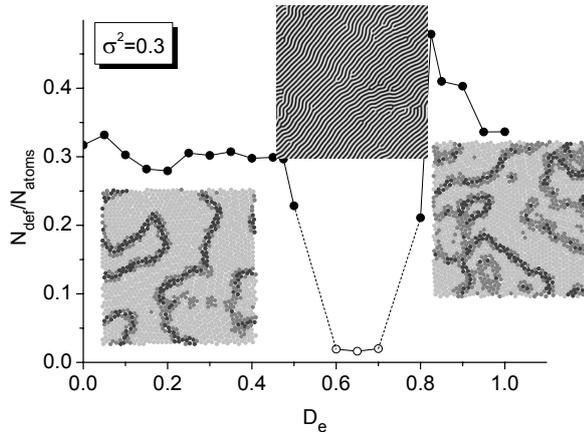


Fig. 9. Dependence of the relative number of defects, $N_{\text{def}}/N_{\text{atoms}}$, on the ballistic mixing intensity D_e at $\sigma^2 = 0.3$, and typical patterns of stationary structures (different shades of gray color correspond to different geometrical imperfections of particles (atoms))

correlation properties of external noise and its competition with the regular component of the ballistic flux substantially affect the changes in the microstructure of crystalline systems and stimulate a structural transformation in them with the emergence of a stationary structure that considerably differs from the structure in the initial crystal.

4. Discussion

The results of our research demonstrate that the hexagonal structure of an initial crystal with stacking faults can undergo modifications owing to the action of the athermal flux. In this case, the spatial distribution of the atomic density may correspond to metastable structures (mixed structures or stripes), which relax into their “equilibrium” configurations (the hexagonal phase) after this flux having been switched off. For the system to transit from the metastable state into the most energetically favorable one, which corresponds to the global minimum of the free energy functional $\mathcal{F}[x]$, thermal fluctuations ξ are needed, which would provide such a transition. Provided that the intensity of such fluctuations is sufficiently high, the transition may be realized within a short time interval. It is this scenario that is observed at a weak external noise, irrespective of the D_e intensity value (small or large). However, if the internal noise intensity ξ is low, the time needed for such a transition to terminate may grow substantially. This circumstance is connected with the depth of a local minimum of the functional $\mathcal{F}[x]$ and the character of the interaction between atoms driven by an external influence. When lin-

ear structures (stripes) are formed, in which the atomic densities of neighbor atoms overlap, the corresponding atoms become bound much more strongly in comparison with atoms in the hexagonal phase. Therefore, for the stripe configuration to be able to transform into the initial hexagonal phase, the system must be heated up substantially by elevating its temperature θ (and the intensity of internal fluctuations, which is proportional to θ). In our case, the evolution of the system was observed only after the athermal flux had been switched off, whereas the temperature did not change. Therefore, although the linear structures obtained at a weak internal noise are stationary, they correspond to a metastable phase (to a local minimum in the free energy functional). Evidently, if we heat the system by raising θ and then cool it down to the initial temperature, we should obtain the initial hexagonal structure of the crystal.

An important issue for the interpretation of the phase with linear structures is their physical meaning. From the results of our research, it follows that the atomic density in them is smeared over the atomic planes separated by the interatomic distance a . To elucidate the physical picture of their formation, the three-dimensional case should be analyzed, in which the bcc structure is a counterpart of the two-dimensional hexagonal phase. Then, since the distance between the nearest neighbors in the bcc structure amounts to $a\sqrt{3}/2$, atoms have the largest overlapping of their atomic densities in the [111] direction, whereas they are separated by the distance a in other directions, so that atomic planes are formed. Hence, the two-dimensional stripes correspond, in effect, to the overlapping of atomic densities in the [111] direction of the three-dimensional system. Actually, it is associated with the correlation noise contribution $D_e\sigma^2C(0)\nabla^2x$, which enlarges the radius of the interaction between atoms. For instance, if we change to the effective flux $\mathbf{J}_{\text{eff}} = -\nabla\delta\mathcal{F}_{\text{eff}}[x]/\delta x$, which makes allowance for both the thermally induced and athermal fluxes, we can write down the functional of effective free energy for the whole system in the form

$$\mathcal{F}_{\text{ef}}[x] = \int \mathbf{dr} \left(\frac{1}{2}x\hat{\varepsilon}(\nabla^2)x + \frac{x^4}{4} + \frac{D_e\sigma^2C(0)}{2}(\nabla x)^2 \right),$$

where $\hat{\varepsilon}(\nabla^2) \equiv \varepsilon_{\text{eff}} + \mathcal{L}(\nabla^2)$, ε_{eff} looks like Eq. (11), and $\mathcal{L}(\nabla^2)$ defines the crystalline order. By analogy with the Cahn–Hilliard theory, the effective radius of the spatial interaction caused by the action of an external source is characterized by the component proportional to $\sqrt{D_e\sigma^2C(0)}$. Hence, the external noise favors the increase of the atom-to-atom interaction radius, thus promoting the overlapping between the atomic densities in

the [111] direction. In such a case, the hexagonal two-dimensional structures are a projection of the bcc crystal cross-section by the (111) plane onto the (000) one – in our case, it is the (x, y) plane – whereas stripes correspond to c projection of the atomic density smeared in the [111] direction onto this plane.

5. Conclusions

In the framework of the phase field crystal method, the simulation of processes leading to microstructural changes in crystalline systems under irradiation, which are associated with a contribution of a stochastic athermal mixing flux, has been carried out. It is found that, in the course of irradiation, the crystalline structure melts at defects belonging to the grain boundaries. At the same time, the correlated action of the stochastic component of the ballistic flux competes with the regular component and promotes the retention of the ordered configuration in the crystal. The study of the recrystallization that takes place after the irradiation has showed that the excited system transforms into a steady state characterized by a small number of point-like and linear defects. It is found that, in the stationary regime, the noise of an external flux can induce the formation of periodic atomic density distributions in space, with the atomic density being smeared over the atomic planes in the dense packing direction. Such structures, although being metastable, are stationary owing to the strong interaction between atoms with overlapped densities. The transition into the initial equilibrium crystalline configuration becomes possible only provided that the temperature of the system is elevated.

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МОДЕЛЮВАННЯ ЗМІНИ МІКРОСТРУКТУРИ
ОПРОМІНЮВАНИХ СИСТЕМ МЕТОДОМ
ФАЗОВОГО ПОЛЯ КРИСТАЛА

Д.О. Харченко, В.О. Харченко, С.В. Кохан, І.О. Лисенко

Резюме

Проведено дослідження зміни мікроструктури систем, підданих дії балістичного потоку, що описує формування структурного безладу при опроміненні із використанням методу фазового поля кристала. Виявлено, що внаслідок конкуренції регулярної та стохастичної компонент балістичного потоку в системі можливе формування структур з розмитими атомними густинами. Проведено дослідження динаміки дефектів при рекристалізації такої системи та встановлено характер зміни кількості дефектів залежно від статистичних властивостей балістичного потоку. Встановлено, що при рекристалізації просторові структури, сформовані під час дії такого потоку, є стаціонарними і стійкими до термічних флуктуацій малої інтенсивності.