MONTE-CARLO MODELING FOR UNSTABLE PARTICLE ENSEMBLES WITH THERMAL FLUCTUATIONS

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In this presentation we study binary alloy systems subjected to particle irradiation and thermal noise influence. We discuss two competing mechanisms of the system evolution: dynamics driven by irradiation and stochastic influences bringing the system toward thermal equilibrium. Using a phase-field formalism and Monte-Carlo modeling we consider self-organization processes in binary alloy systems with field/concentration dependent mobility/diffusion coefficient. Generalization of the phase separation scenario and patterning in such systems are presented.

1. INTRODUCTION

It is well known that the sustained irradiation of materials produces a disorder which can be structural (isolated point defects, traps, dislocation loops, clusters of vacancies and interstitials). Such point defects in alloys are considered as unstable particles which can exist for some fixed lifetime and can lead to self-organizational processes: if its density is large, then the interaction processes start to play a crucial role leading to a new phase appearance caused by collective effects. If the above disorder is continuous then a net flux of defects can be induced that results in driving the material into stationary non-equilibrium states. For irradiation processes that occur at finite temperature a thermally activated dynamics leads to annealing such non-equilibrium disorder. Therefore, the question which is of fundamental interest is to study competing dynamics caused by regular and irregular forces leading to microstructural change in such materials. It is known that dynamical systems often reach some steady state (quasi-steady state in the case of alloys under irradiation), and one appealing approach is to develop an effective theoretical and thermodynamical framework to address the stability of these steady states.

Usually, to investigate such non-equilibrium phenomena one can exploit multi-scale modeling: molecular dynamics (MD) methods or kinetic Metropolis procedures that allow one to find statistical information that can be transferred to the next hierarchical level of calculation, namely kinetic Monte-Carlo (KMC). The principle idea lies in the fact that on atomic length ($\sim 10^{-10}$ m) and time scales ($\sim 10^{-13}$ s) the system dynamics can be captured by MD. Unfortunately, the number of atoms in MD simulations is still small ($\sim 10^{9}$ atoms), the time interval for predictions of MD simulations is too short ($\sim 10^{-8}$ s) to describe microstructure transformations on a atomic length scales and mesoscopic time scales [1]. The problem can be partially solved by KMC. The principle idea of the original KMC can be stated as follows: given a system and its phase space, a distribution of configuration at initial (starting) time, and a set of transition rates between configurations, one can generate temporal trajectories of the system in its phase space. Such trajectories should be produced by correct statistical weight. Both the average evolution of the system and its fluctuations around this average can be obtained from a large set of temporal trajectories. From the mathematical viewpoint the problem is to solve the numerically master equation of the Chapmen-Kolmogorov's kind. This method has some limitations because one needs to calculate all possible macroscopic transition rates in one time step.

Progress that alleviates this limitation has been made recently by the introduction of the phase field theory adapted to description of crystals [2]. Using this method one can consider a local atomic density field in which atomic vibrations have been integrated out up

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to diffusive time scales. Therefore, dissipative dynamics is governed by the temporal evolution such local density field. Deterministic dynamics can be generalized introducing stochastic sources into the corresponding evolution equations. As usual, fluctuating sources represent statistical information about the influence of microscopic processes onto mesoscopic ones. Considering alloys under irradiation, such fluctuating sources can be divided by its physical character: thermal fluctuations obeying the fluctuation-dissipation relation and external noise addressed to local dynamics driven by irradiation caused by energetic particles, some transformation of defects, chemical reactions, etc. Such KMC simulations allow one to investigate the role of fluctuating sources on microstructural transformations of alloys under irradiation, and to predict the system behavior under fluctuating sources influence. Despite some useful advantages of this method, one needs to highlight that due to the diffusive time scales considered this method does not contain a mechanism to simulate elastic interactions to study deformation properties of alloys.

Returning back to the main question noted above, one needs to say that in the case of alloys under particle irradiation, in order to describe the non-equilibrium steady states and the corresponding system behavior one needs to construct an associated non-equilibrium potential/functional to find a stationary distribution. If such a functional can be found exactly, then one can describe local physical fields such as concentration deviation, local magnetization, polarization in real space, and thus investigate their spatial profiles. Considering the related problem of irradiation of alloys, this can be shown to be a consequence of patterning which in turn is a result of the competing dynamics between two of the above noted dynamics [3]. Formation of patterns of anti-structure defects induced by irradiation, was studied in [4]. It was shown that under irradiation stable and unstable configurations of anti-structure defects can be observed. The authors explain that at a fixed irradiation dose an increase in the temperature leads to a transition from unstable into stable ordered configurations. Some attempts to study the influence of fluctuation terms on microstructure transformations were recently reported [5,6]. It was shown that in binary alloys under irradiation a macroscopic phase separation manifested as a patterning can be observed (see for example [7-9]). In these works the authors studied systems when the dynamical governing equation is identical to that describing a binary alloy undergoing a quasi-chemical reaction A↔B with phase separation processes. The term related to such a quasi-chemical reaction (local force) was assumed to be linear (Debye relaxation processes) and to describe ballistic mixing or birth-death processes for unstable particle ensembles. It was shown that by controlling the irradiation intensity one arrives at different regimes of the system's behavior: patterning, macroscopic phase separation, and solid solution.

In this paper we discuss a similar model reduced to the quasichemical reactions in alloys A↔B that occur with the help of additional product (Schlögl model for fluctuations in moving fronts between two phases: A+2X↔3X, X↔B). Such a model can be obtained directly from the dynamical approach if the possible stationary states are well known. It is possible then to describe clustering and dissociation effects caused by irradiation. In addition we introduce into the model a flux of a local atomic density and a fluctuating source obeying a fluctuation-dissipation relation. Moreover, we assume that mobility, related to the diffusion coefficient, is a field-dependent function that leads to the fact that our fluctuating force is also field-dependent function. We will show that under such noise influence the system can undergo phase separation, patterning with different kinds of structures: bubbles/porous, spinodal decomposition, and strip patterns with dislocations. Our analytical investigation is compared with computer simulations and verified with well known results of phase modeling of alloys under irradiation.

2. GENERALIZED MODEL

We study the problem using a Cahn-Hillard-type description of fronts, allowing us to simulate the walls of the labyrinthine patterns. The equation describing the temporal evolution of the concentration field $x=x(\mathbf{r},t)$ is

composed of two terms, one for mixing caused by irradiation (relocation of atoms), and another one for thermal diffusion. Formally, such a reaction-diffusion model can be described by the generalized continuity equation of the form

$$\partial_t x = f(x) - \nabla \cdot J, \qquad (1)$$

where *f(x)* stands for the local dynamics, and *J* is the flux for transport phenomena. Considering the non-Fickian diffusion, we exploit a gradient of interaction potential $U(\mathbf{r})$ ($U(\mathbf{r}) = -\int u(\mathbf{r}-\mathbf{r}')x(\mathbf{r}')d\mathbf{r}'$, where the spherically symmetric interaction potential $u(\mathbf{r})$ between particles separated by a distance $|\mathbf{r}|$ is introduced). The corresponding force given by the gradient of $U(\mathbf{r})$ governs the transport phenomena. In the case of the small interaction radius compared to the diffusion length the concentration field *x* will not vary significantly within the interaction radius. It allows us to approximate the integral by $\kappa x+\beta\Delta x$, where

$$\int u(\mathbf{r})d\mathbf{r} = \kappa; \quad \int \mathbf{r}u(\mathbf{r})d\mathbf{r} = 0;$$

$$\frac{1}{2}\int |\mathbf{r}|^2 u(\mathbf{r})d\mathbf{r} = \beta \approx \frac{1}{2}\kappa r_c^2;$$

r_c is a correlation radius. Therefore, the obtained flux allows one to describe phase separation processes with mutual (lateral) interactions; the combined model with local dynamics can be used to consider the spatial patterns induced by the fluctuations of the bath.

Generally, the local dynamics is defined by a force assumed to be of the form $f(x) = dV(x)/dx$, where the local potential is assumed as $V(x) = -\varepsilon x^2/2 + \mu x^3/3 + x^4/4$. Here ε and μ are control parameters related to rates of quasi-chemical reactions in the system. For the diffusion flux one use the definition: $J = -D(x)\nabla\delta F/\delta x$, where *D(x)* is a field-dependent diffusion coefficient, and the free energy functional is of the from $F = \int dr[-\kappa x^2/2 + \beta(\nabla x)^2/2]$, related to the lateral interactions between particles. For the diffusion coefficient we will use an approximate formula describing a bell shaped form of *D* versus the atomic density field, i.e. $D(x) = (1+\alpha x^2)^{-1}$. Such the approximation is widely used in the study of phase separation dynamics in a large class of physical systems. The parameter α is usually reduced to the ratio between bulk and surface diffusion coefficients ($\alpha \approx 1\text{-}D_b/D_s$).

Considering the system under real conditions, one needs to introduce fluctuating source related to the problem under consideration. Formally, such fluctuations can be included in an *ad hoc* form. Using variational principles one can rewrite Eq.(1) in the form $\partial_t x = -[D(x)]^{-1}\delta\Lambda/\delta x$, where Λ is a Lyapunov's functional related to the right hand side of the Eq. (1):

$$\delta\Lambda = -\int dr\delta x[f(x)D(x) + D(x)\nabla(D(x)\delta F/\delta x)].$$

Next we introduce Gaussian fluctuations ζ into such an equation in order to satisfy the fluctuation-dissipation relation

$$\langle\zeta(x;r,t)\zeta(x;r',t')\rangle = [D(x)]^{-1}\sigma^2\delta(r-r')\delta(t-t'),$$

σ^2 is the noise intensity reduced to the temperature of the effective bath; $\langle\zeta(x;r,t)\rangle = 0$. As a result we arrive at a stochastic evolution equation for the mass density field in the form

$$\frac{\partial x}{\partial t} = -\frac{1}{D(x)}\frac{\delta\Lambda}{\delta x} + \zeta(x,r,t) \qquad (2)$$

treated in the Stratonovich sense. This equation can be used to provide KMC simulations of dynamical regimes of the system. Statistical properties of the system states can be found from the stationary picture that is described by the corresponding stationary distribution, following from the stationary solution of the Fokker-Planck equation. Performing the standard calculations one arrives at the distribution functional in the form

$$P[x] \propto \exp(-U_{ef}[x]/\sigma^2),$$
$$U_{ef}[x] = \Lambda[x] - \frac{\sigma^2}{2}\int dr \ln D(x). \qquad (3)$$

It follows, that the stationary distribution functional *P*[*x*] or the effective functional $U_{ef}[x]$ are obtained exactly: the form of initial functional Λ[*x*] is supposed to be known, the second term in $U_{ef}[x]$ can be calculated if needed. Let us note, if we assume that Λ[*x*] plays a role of an effective free energy functional, then rewriting the integral in Eq. (4) as $S_{ef} = \frac{1}{2}\int dr \ln[D(x)]^{-1}$, the expression

for $U_{ef}[x]$ can be transformed into the thermodynamic relation between free energy, internal energy and entropy functionals: $U_{ef}[x]=\Lambda[x]+S_{ef}[x]$. Therefore, according to such a relation the noise intensity σ^2 reduces to an effective temperature of the bath, whereas $S_{ef}[x]$ plays the role of an effective entropy. Such a situation is well known in stochastic systems theory. It appears when the multiplicative fluctuations corresponded to the internal noise. The later one results in the entropy change that yields entropy driven phase transitions [10-13]. In this paper we will not discuss the above phase transitions, but we will consider the ability of the noise to sustain or induce formation of spatial structures.

3. RESULTS

3.1. Internal noise influence on the phase separation scenario

Firstly, let us consider the generalized approach based on the Cahn-Hillalrd-type theory allowing us to describe a phase separation scenario of a microstructure transformation. Here we assume that no quasi-chemical reactions are possible, i.e. $f(x)=0$, the free energy functional $F[x]$ is assumed in the Ginzburg-Landau form, i.e.

$$F = \int dr[-\varepsilon x^2/2 + x^4/4 + \beta(\nabla x)^2/2].$$

Therefore, an evolution of the concentration field $x=x(\mathbf{r},t)$ is governed by the Langevin equation of the form

$$\partial_t x = \nabla \cdot \left(D(x)\nabla \frac{\delta F[x]}{\delta x} \right) + \nabla\sqrt{D(x)}\xi(\mathbf{r},t), \quad (4)$$

where $\langle \xi(\mathbf{r},t)\xi(\mathbf{r}',t')\rangle = \sigma^2\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$, and $\langle \xi(\mathbf{r},t)\rangle = 0$. Statistical properties of such a system can be described by the probability density functional $P[x]$, that can be exactly found as a solution of the corresponding Fokker-Planck equation. It was shown that such a functional is of the form [14]

$$P[x] \propto \exp(-U_{ef}[x]/\sigma^2),$$
$$U_{ef}[x] = F[x] + \frac{\sigma^2}{2}\int dr \ln D(x). \quad (5)$$

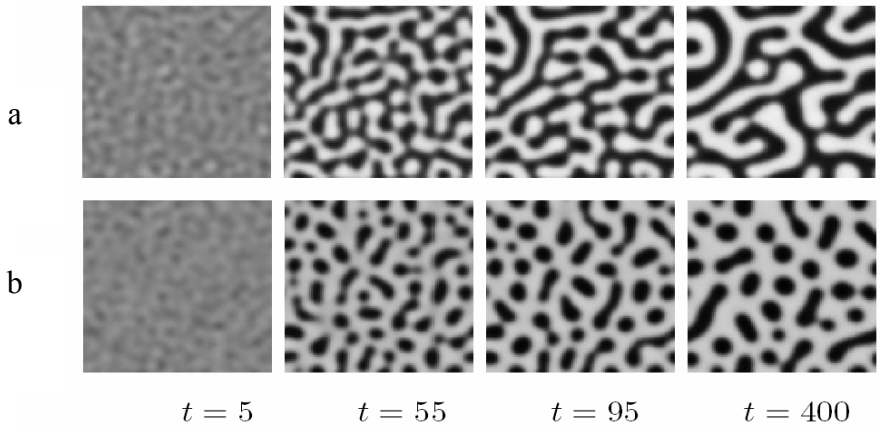

Fig. 1. Typical spatial patterns as a solution of the Langevin equation on a regular 2-dimensional lattice of $N=L^2$, $L=120$: a - spinodal decomposition; b - nucleation. Other parameters are: $\beta=4$, $\varepsilon=1$, $\alpha=0.5$, $\sigma^2=0.2$

In such kinds of stochastic models, the scenario of the phase separation depends on the initial conditions: at $\langle x(\mathbf{r},0)\rangle = 0$ the system evolves by a spinodal decomposition scenario (see Fig. 1,a), whereas at $\langle x(\mathbf{r},0)\rangle \neq 0$ a nucleation process is realized (Fig. 1,b). In further investigation herein, we will study only the spinodal decomposition.

Next, let us consider the early stages of the system's evolution. To this end we calculate the structure function $S_{\mathbf{k}}(t) = \langle x_{\mathbf{k}}(t)x_{-\mathbf{k}}(t)\rangle$, in the vicinity of the mixed state $x=0$, where $x_{\mathbf{k}} = (2\pi)^{-d}\int x(\mathbf{r})e^{-i\mathbf{kr}}d\mathbf{r}$. In the framework of a linear stability analysis we obtain the

evolution equation for the structure function in the form

$$\frac{1}{2}\frac{d}{dt}S_{\mathbf{k}}(t) = -k^2(\beta k^2 - \varepsilon + \alpha\sigma^2)S_{\mathbf{k}}(t) + \sigma^2 k^2 - k^2\frac{\sigma^2}{(2\pi)^d}\int S_{\mathbf{q}}(t)d\mathbf{q} \quad (6)$$

from which it follows that the fluctuating source does not lead to instability of the mixed/disordered state. From exponential solutions of Eq. (6) one can see that only modes with $k < k_c = \sqrt{2d(\varepsilon - \alpha\sigma^2)/D}$ are unstable and grow at early stages of evolution. With an increase in α or σ^2 the size of the unstable domain modes $k<k_c$ decreases. Modes with $k>k_c$ remain stable during the linear regime. One needs to stress that the unstable modes cannot be realized at the condition $\varepsilon<\alpha\sigma^2$. As it follows, the domain growth should be different for additive and multiplicative nois.

In Fig.2 we present solutions of the evolution equation (6) at different values of the parameter α. It can be seen that an increase in α leads to a shift of the peak position toward smaller values of *k*. The peak of *S(k)* is less pronounced in the multiplicative noise case than in the case of the additive noise. It follows that, if the multiplicative noise is considered, then the dynamics is slowed. A decrease in the peak height means that the interface is more diffuse in the case of multiplicative noise (see insertions in Fig.2).

We compare analytical results with computer simulations at the same time *t* in the two-dimensional lattice. In the insertions of Fig. 2 typical patterns and images of spherically averaged structure functions are shown. It is seen that in the multiplicative noise case the pattern has a more diffuse interface and the resonance ring in *S(k)*-dependence is less pronounced than for the additive noise.

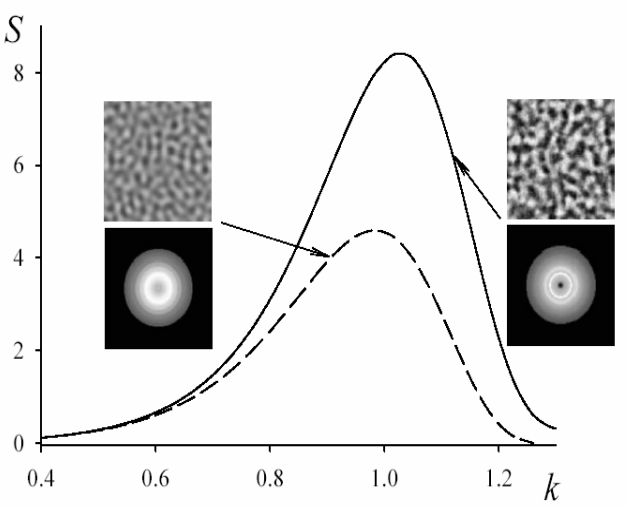

Fig. 2. Evolution of the structure function at an early stage t=10 at β=4, ε=1, σ^2=0.3. Different values of the parameter α are used to compare the influence of additive α=0 and multiplicative α=0.9 noises (solid and dashed lines, respectively). Insertion shows typical patterns and corresponding images of spherically averaged structure functions at the same time obtained from numerical solutions of Eq.(4) at x^3

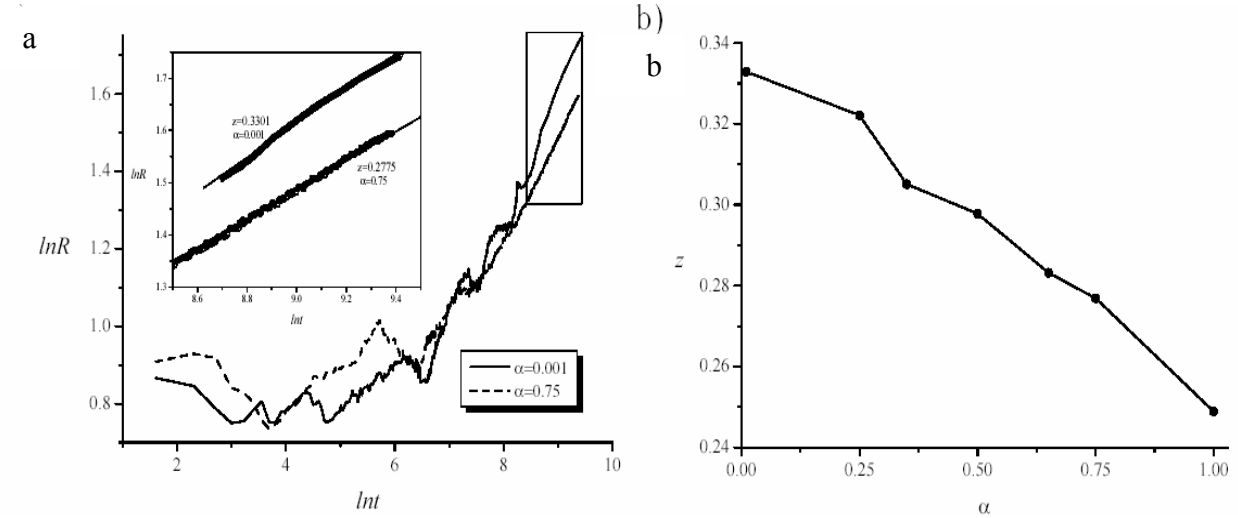

Fig. 3. Power law for domain size growth: a - log-log plot of the evolution of R(t) at different values of the parameter α (insertion shows universal behavior of the function R(t) at large times, indicated in the rectangle); b - dependence of the power law exponent z versus parameter α. Other parameters are ε=1.0, β=4.0, σ^2=0.2

At late stages of the system's evolution one can estimate in what manner such thermal fluctuations can modify the domain size growth law. In order to obtain the linear domain size growth law *R(t)* we use following relations:

$$R(t) = \langle k(t) \rangle^{-1}; \qquad \langle k(t) \rangle = \frac{\int_0^{k_{\max}} S(k,t) k dk}{\int_0^{k_{\max}} S(k,t) dk}, \qquad (7)$$

where in this calculation we have used the spherically averaged structure function *S(k,t)* [10]. The power law behavior of the function $R(t) \propto t^z$ is verified at different values of the parameter α, where the domain growth exponent depends on α, i.e. *z=z(α)* (see Fig. 3). It is seen that in the case of additive noise (α=0) the exponent $z \approx 1/3$, whereas at α=1.0 we obtain $z \approx 1/4$. Therefore, with an increase in α, a crossover of dynamical regimes is observed. Our results are in good correspondence with deterministic and stochastic approaches which indicate that an increase in the parameter α delays the dynamics [15-17]. Comparing our results with results related to phase separation regimes in alloys under irradiation, one can conclude that with an α increase the crossover from strong- to weak-segregation regimes can be realized [7].

3.2. Patterning scenario under irradiation and fluctuating source influence

In this subsection we discuss the influence of internal noise on the pattern formation scenario in systems under irradiation. To this end we assume that there is a local dynamics caused by the irradiation, described by the force *f(x)*. Moreover, we assume that the thermal diffusional processes are possible. The latter is described by non-Fickian diffusion with interaction potential *U(r)*. Introducing the corresponding fluctuating source into the evolution equation for the concentration field, the probability density functional takes the form of Eq. (3). At first let us investigate the structure of the effective potential considering a homogeneous (zero-dimensional) system where the mass density field does not depend on the spatial coordinate. To find the homogeneous solutions we need to compute the extrema positions of the function $U_{ef}(x)$ when the noise intensity is changed, and calculate the corresponding phase diagram, illustrating the change in the number of extrema of the function $U_{ef}(x)$.

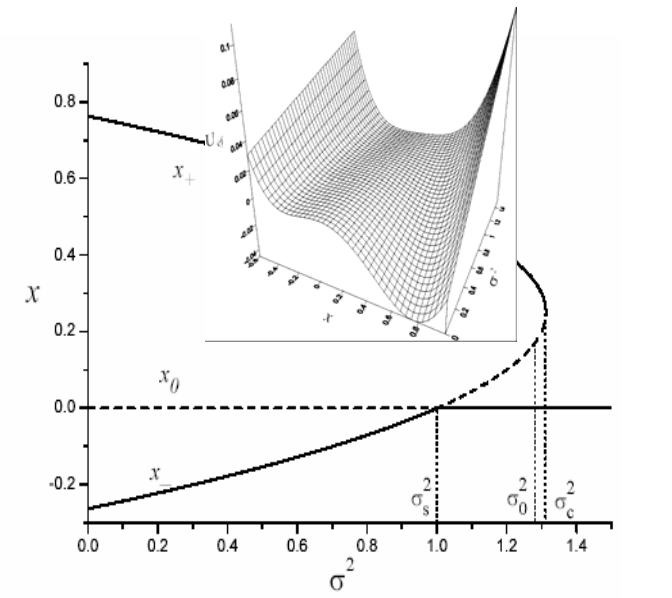

Fig. 4. Bifurcation diagram for noise induced transitions (a change number of extrema of the function $U_{ef}(x)$) at α=0.2, ε=0.2, μ=-0.5. Solid lines define stable states, the dashed line corresponds to the unstable solution. The form of the effective potential is shown in insertion

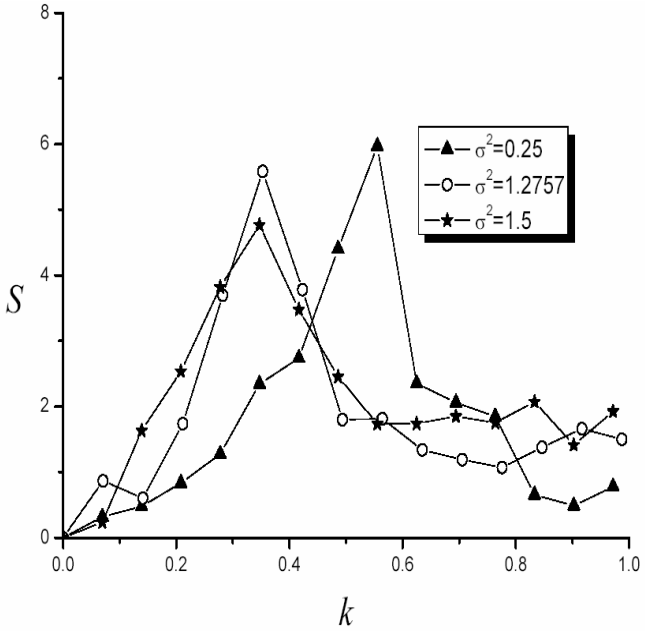

Fig. 5. An averaged structure function at different values of the noise intensity at t=4000 (the model of lateral interactions): triangles correspond to $\sigma^2=0.25$; circles correspond to $\sigma^2=\sigma_0^2$; and stars relate to $\sigma^2=1.5$. Other parameters are: ε=0.2, μ=0.5, κ=1.0, β=1.0, and α=0.2

In our investigations we assume that our effective concentration field can take values in the interval [-1,1] to describe two possible dense phases, whereas for the mixed one it corresponds to x=0. To consider a case $x \in [-1,1]$ let us assume values of both ε and μ to locate a minimum $U_{ef}(x\_)$ at x<0, a minimum $U_{ef}(x_+)$ we locate at x>0. An appropriate choice is ε=0.2, μ=-0.5, α>0. The corresponding dependencies $x_{\pm}(\sigma^2)$ are shown in Fig. 4. To understand transformations of the system states let us use the noise induced transitions formalism [18]. As it follows from naive considerations, the bimodal stationary distribution $P_{st}(x) \propto \exp(-U_{ef}(x)/\sigma^2)$ becomes unimodal with an increase in the noise intensity. In the case under consideration here, the transition occurs in the following manner. In the noiseless case, a form of the effective potential U_{ef} is topologically identical to a form of the initial potential $V(x)$. With an increase in the noise intensity a minimum of U_{ef} located at $x\_$ tends to zero, at $\sigma^2 = \sigma_s^2 = \varepsilon/\alpha$ the effective potential has a double degenerated point, x_0=$x\_$=0. Therefore, the values σ_s^2 define a spinodal curve. At $\sigma_s^2 < \sigma^2 < \sigma_0^2$ the point x_0 relates to a minimum, whereas $x\_$ defines a maximum position of the function U_{ef}. These two minima differ in depth. At $\sigma^2 = \sigma_0^2$ one has $U_{ef}(0)=U_{ef}(x_+)$, therefore, σ_0^2 defines a coexistence line (binodal). With a further increase in the noise intensity we get $U_{ef}(0)<U_{ef}(x_+)$. At $\sigma^2 = \sigma_c^2 = \alpha^{-1}(\varepsilon + \mu^2/4)$ one gets another spinodal. At $\sigma^2 > \sigma_c^2$ the effective potential has one well only. Therefore, in such a noise induced transition we have a shift of the potential extreme, transformation of the global minimum into a local one, loss of its stability and, finally, a change in the number of extrema of the function U_{ef}. To analytically study a possibility of patterning in the system under consideration, one needs to solve a variational problem $\delta U_{ef}/\delta x = 0$. Indeed, the stationary structures $x(\mathbf{r})$ should correspond to extrema positions of the effective functional $U_{ef}[x]$. Solutions of the corresponding variational problem allows one to find the stable structures that are formed in the vicinity of the positions' of local minima of the effective potential $U_{ef}(x)$. The corresponding stationary profiles of the most probable concentration field $x(\mathbf{r})$ obtained, have one period only. This result is verified by a numerical solution of the Langevin equation (2) where the spherically averaged structure function has only one peak (see Fig. 5).

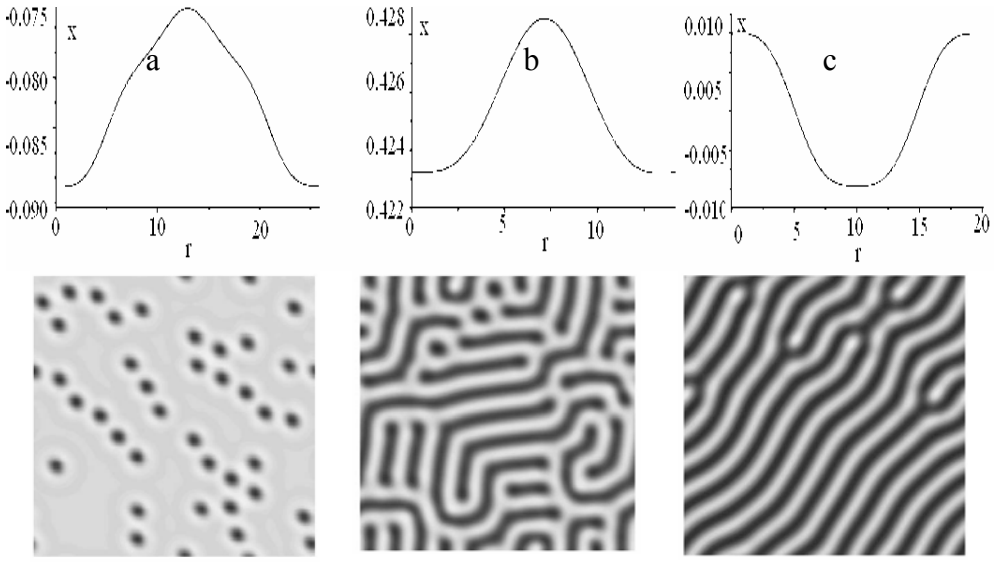

Fig.6. One dimensional concentration profiles (top) and two-dimensional stationary patterns at σ^2=0.2 (a), $\sigma^2 = \sigma_0^2$ (b) and σ^2=2 (c). Other parameters are: α=0.2, ε=0.2, μ=-0.5, β=1.0, κ=1

The corresponding simulations of spatial patterns in a two-dimensional lattice allows one to find that at small noise intensities $\sigma^2 < \sigma_s^2$ the system is organized in patterns of the type "vacancy clusters" with very small values of the concentration field (see Fig. 6, a). At $\sigma^2 = \sigma_0^2$ when two minima of the effective potential $U_{ef}(x)$ located at $x=0$ and $x=x_+$ are equivalent in depth, a condition of phase separation is realized (Fig.6, b). Here the average concentration $x(\mathbf{r},t)$ is the constant value (conserved dynamics), but there is no domain size growth law, as is realized in phase separation processes (see Sec.3.1). Here, the linear size of the domain R saturates and does not grow in time, it decreases with σ^2 as $R(\sigma^2) \propto (\sigma^2)^{-1.6\pm0.01}$. At large noise intensities $\sigma^2 > \sigma_c^2$ the system is organized into strip phases with liner defects of the dislocation type (Fig. 6, c). It is interesting to note that at noise intensities $\sigma^2 > \sigma_T^2 = \sigma_s^2 + \kappa^2/4\alpha$ fluctuations destroy the stable ordered patterns and stable structures can not be formed. Patterns cannot be formed if irradiation effects are not considered.

4. CONCLUSIONS

We have discussed the possibility of phase separation processes and pattern formation in stochastic systems such as binary alloys under irradiation conditions. We have examined the phase separation scenario of the system with internal multiplicative noise related to the field-dependent mobility. Analysis was performed for early and late stages of the evolution by computer simulations. We have generalized the well known results of phase separation theory. Comparing the noise induced transition picture and pattern formation processes, it was shown that the system follows the entropy driven mechanism by analogy with entropy driven phase transition theory. Our study shows that at a small noise intensity the system manifests a nucleation regime, at fixed values of the noise strength a spinodal decomposition is realized, and at large noise the system exhibits strip patterns with liner defects. Strip structures exist in the fixed interval of the noise intensity – large fluctuations destroy patterns.

The obtained results can be applied to study patterns in adsorption/desorption processes in metal deposition of a monolayer of molecules and in processes of microstructure transformations of materials subject to intensive irradiation.

REFERENCES

1. J. Chang, W. Cai, V.V. Bulatov, S. Yip // *Comp. Mat. Sci*. 2002, v. 23, p. 11.
2. K.R. Elder, M. Katakowski, M. Haataja, M. Grant // *Phys. Rev. Lett.* 2002, v. 88, p. 245701.
3. G. Martin // *Phys. Rev B*. 1984, v. 30, p. 1424; V.G. Vaks, V.V. Kamyshenko // *Phys. Lett. A*. 1993, v. 177, p. 269.
4. В.В. Михайловский, К.С. Расселл, В.И. Сугаков // *ФТТ*. 2000, v. 42, №3, p. 471.
5. V.I. Sugakov // *Sol. State Commun*. 1998, v. 106, p. 705.
6. R.A. Enrique, P. Bellon // *Phys. Rev. B*. 2004, v. 70, p. 224106.
7. R.A. Enrique, P. Bellon // *Phys. Rev. Lett.* 2000, v. 84**,** N 13, p. 2885.
8. Ji wen Liu, P. Bellon // *Phys. Rev. B*. 2002, v. 66, p. 020303(R).
9. R.A. Enrique, P. Bellon // *Phys.Rev B*. 2004, v. 70, p. 094104.
10. M. Ibanes, J. Garcia-Ojalvo, R. Toral, et al. // *Phys.Rev.Lett.* 2001, v. 87, p. 020601.
11. B.von Haeften, G. Izus, S. Mangioni, et al. // *Phys. Rev. E*. 2004, v. 69, p. 021107.
12. J. Buceta, Kevin Wood, Katja Lindenberg // *Phys. Rev. E*. 2006, v. 73, p. 042101.
13. D.O. Kharhcenko, A.V. Dvornichenko // *Eur. Phys. Jour. B*. 2008, v. 61, p. 95.
14. D.O. Kharhcenko, A.V. Dvornichenko // *Physica A*, be published.
15. I.M. Lifshitz, V.V. Slyozov // *J. Phys. Chem. Solids*. 1961, v**.** 19**,** p. 35.
16. C.L. Emmott, A.J. Bray // *Phys. Rev. E*. 1999, v. 59, p. 213.
17. J.M. Sancho, A. Hernandez-Machado, L. Ramirez-Piscina, A.M. Lacasta // *Acta Phys. Polonica B*. 1993, v. 24, p. 733.
18. W. Horsthemke, R. Lefever. *Noise-Induced Transitions*. Springer-Verlag, Berlin, 1984.

СТАТИСТИЧЕСКОЕ МОДЕЛИРОВАНИЕ АНСАМБЛЕЙ НЕСТАБИЛЬНЫХ ЧАСТИЦ С ТЕПЛОВЫМИ ФЛУКТУАЦИЯМИ

Д.О. Харченко

Исследуются системы бинарных сплавов, подверженных облучению частиц и воздействию тепловых шумов. Обсуждаются два конкурирующих механизма эволюции системы: динамика, вызванная облучением, и стохастические воздействия, переводящие систему к тепловому равновесию. С использованием формализма теории фазового поля и статистического моделирования рассматриваются процессы самоорганизации в системах бинарных сплавов с подвижностью, зависимой от поля концентрации. Предложено обобщение сценария фазового расслоения и структурообразования в таких системах.

СТАТИСТИЧНЕ МОДЕЛЮВАННЯ АНСАМБЛІВ НЕСТАБІЛЬНИХ ЧАСТОК З ТЕПЛОВИМИ ФЛУКТУАЦІЯМИ

Д.О. Харченко

Досліджуються системи бінарних сплавів, підданих опроміненню часток і впливу теплових шумів. Обговорюються два конкуруючих механізми еволюції системи: динаміка, обумовлена опроміненням і стохастичні впливи, що переводять систему до теплової рівноваги. З використанням формалізму теорії фазового поля і статистичного моделювання розглядаються процеси самоорганізації у системах бінарних сплавів з рухомістю, яка залежить від поля концентрації. Запропоноване узагальнення сценаріїв фазового розшарування і структуроутворення у таких системах.