Nonlinear Dynamics and Applications

27

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Minsk 2021

Proceedings of the Twenty-eight Anniversary Seminar NPCS'2021
in memory of Prof. V.I. Kuvshinov
May 18-21, 2021, Minsk, Belarus
Fractals, Chaos, Phase Transitions, Self-organization

Editors
V.A. Shaparau
A.G. Trifonov

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Preface

The 28th Anniversary International Seminar "Nonlinear Phenomena In Complex Systems" was held in memory of Prof. V.I. Kuvshinov on May 18-21, 2021, in Minsk, Belarus.

The bright memory of

Vyacheslav Ivanovich Kuvshinov

will forever remain in our hearts.

The 28th Anniversary International Seminar traditionally had subsubjects: "Fractals, Chaos, Phase transitions, Self-organization", plenary session and the following section sessions: Particles, Modelling and Safety Related Analyses of NPP, Quantum and Classical Electrodynamics, Gravity, Media, Medicine, Biological and Chemical systems, Mathematics and Fields. 14 plenary, 48 section and 7 poster reports were submitted to the 28th Seminar by the scientists. At this Anniversary Seminar, the participants gave overview reports, which became useful to young scientists. Thus, in addition to the scientific component, the seminar also played an educational role. Most of the papers were included into these Proceedings.

The 28th Anniversary Seminar 'NPCS' was supported by National Academy of Sciences of Belarus.

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Finsler-Lagrange Modeling of Langmuir Monolayer Domain Structure at First-Order Phase Transition

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To date, Langmuir monolayer and Langmuir-Blodgett films are considered as a promising material for fabrication of quantum signal transducers in nanoelectronics, nanooptics and nanosensorics. Because of that, the theoretical modeling of the first-order phase transition in the Langmuir monolayer is in great demand. It has been shown that the Langmuir monolayers are characterized by the direction dependent growth of domains that is a result of local non-equilibrium field configurations during domain nucleation at monolayer compression. In the paper we develop the Finsler-Lagrange model of Langmuir monolayer structurization taking into account the relaxation-time distribution of domains. Here, we apply a billiard model to find out the domain shapes on the early stage of nucleation in dependence on monolayer parameters and compression rate. We assume that billiard boards model the interaction of crystal nuclei with monolayer molecules in liquid state, which play a role of local environment.

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Keywords: Langmuir monolayer, first order phase transition, Finsler-Lagrange configuration space, domain growth, Finsler billiards model.

1. Introduction

A series of step-by-step phase transitions from a two-dimensional (2D) gas into 2D crystal state is observed at Langmuir monolayer compression on the surface of a polar liquid [1, 2]. It has been shown experimentally that 2D phase transition from expanded liquid to crystal state depends significantly on the properties of amphiphilic molecules and the monolayer formation conditions, i.e. on an ion composition of a subphase and a compression rate [3–10]. It has been shown in [11] that sharp changes occurs in morphology of crystal phase domains at increase of the compression rate. At low compression rates the round-shape domains are formed during phase transition while at high monolayer compression rates asymmetric fractal-like domain growth has been observed. The theoretical models proposed for Langmuir monolayer description do not demonstrate the

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experimentally revealed dependencies of the phase domain shape [12], of viscosity [13], of temperature and of surface tension [14, 15] on monolayer compression rate at first-order phase transition. Such effects of the compression rate on phase transition dynamic are stipulated by electrocapillary phenomena and by redistribution of charge density of Helmholtz electrical double layer.

The aim of the present paper is to study the domain growth using Finsler mathematical billiard model in the framework of previously developed Finsler-Lagrange geometric theory which accounts electrocapillary effects and phase nuclei relaxation time distribution, .

2. Finsler-Lagrange model

The model under consideration demonstrates the influence of the compression rate on the dynamics of 2D first-order phase transition. Taking into account the relaxation time distribution we study the dynamics of the system in a configuration space $\left(\vec{r},\, \xi,\, \dot{\vec{r}}_{\xi},\, \dot{\xi}_{s},\, s\right)$. Here $\vec{r}$ is a 2D radius vector, $\xi \equiv t$ is a time variable, the dots denote the derivatives on the evolution parameter s. The metric of this space is determined by the pseudo-Finsler metric function of the following form [16, 17].

$$dl^2 = L(\vec{r}, \dot{\vec{r}}, \dot{\xi})ds^2 = -\tilde{p}Vr^5 e^{\frac{2V\xi}{r}}\frac{\dot{\xi}}{\dot{r}}d\xi\, ds + \tilde{U}(\xi, r)\dot{\xi}\, ds^2 + m\frac{(\dot{r}^2 + r^2\dot{\phi}^2)}{2\dot{\xi}}ds^2 \qquad (1)$$

where V is the compression rate; $\tilde{p}$, c and m are model system parameters, the function $\tilde{U}(\xi, r)$ is defined by the potential function.

Domain growth is analyzed as a domain wall movement. On the nucleation stage and early nuclei growth stage of first-order phase transition the particles of the original phase (2D expanded liquid) put the pressure upon the domain-wall of the nucleating phase (2D crystal state). Let us consider the particle-like states as such original phase elements (domains) which do not bound to the growing domain but participate in collisions with the domain wall. These "particles" move along the geodesics of the configuration space-time. The collisions gives the additional entropy Δs into the system. The quantity of Δs can be determined from the visiting set of a probe particle on a some sphere-shaped billiard desk of the initial space. The movement of a probe particle in this round billiard takes place along the geodesics which are associated with the fixed indicatrixes of the pseudo-Finsler configuration space (1).

Further we specify the law of reflection of a particle from the relativistically moving domain wall. Let us consider the particle moving in a circular billiard of the constant radius R. If the boundary is immovable, the reflection law has a simple form in Riemannian spaces: angle of incidence equals to angle of reflection. The configuration space for which the metric is determined as the square of the metric function (1) is pseudo-Finsler one. The metric depends on the velocities $\dot{\xi}, \dot{r}, \dot{\phi}$, the consequence of that is the another law of reflection. It has been shown [18] that the law of reflection can be found by means of geometrized variational principle. It leads to the possibility of construction of the law of reflection using the indicatrixes of Finsler spaces. For Finsler spaces because of the section of the indicatrix is not circular one, the angle of incidence is not equal to the angle of reflection in general. The complicated law of reflection impedes significantly the investigation of the Finsler billiards.

The model of a circular-shape billiard with moving boundary is constructed in the following way. Let consider a mass surface $\dot{\xi} = 1$ in the Finsler space with the metric (1). It has been shown previously [16] that on the mass surface the metric function (1) can be represented as

$$F^2 = -L(\vec{r}, \dot{\vec{r}}, \dot{\xi})\dot{\xi} \equiv A\frac{\dot{\xi}^3}{\dot{r}} + B\dot{\xi}^2 - m\frac{(\dot{r}^2 + r^2\,\dot{\phi}^2)}{2}. \qquad (2)$$

The potential defining the dynamics of the system has a form

$$U(\dot{r},\, r, t) = -p\left[\left(P_1 - r^5\frac{V}{\dot{r}}\right)e^{\frac{2Vt}{r}} - \frac{4}{45}\frac{(Vt)^6}{r}\mathrm{Ei}\left[\frac{2Vt}{r}\right]\right],$$

where

$$P_1 = -\frac{4}{3}r^5 + \frac{16}{15}(V\,t)r^4 + \frac{1}{30}(V\,t)^2r^3 + \frac{1}{45}(Vt)^3r^2 + \frac{1}{45}(Vt)^4r + \frac{2}{45}(Vt)^5.$$

The functions A, B are

$$A = pVr^5e^{\frac{2\,V\,t}{r}}, \qquad B = m^2 - p\left(P_1\,e^{\frac{2\,V\,t}{r}} - \frac{4}{45}\frac{(V\,t)^6}{r}\mathrm{Ei}\left[\frac{2V\,t}{r}\right]\right). \qquad (3)$$

The dynamics is given by the Lagrange-Euler equations:

$$\frac{dy^i}{ds} + 2G^i = 0, \qquad G^i = \frac{1}{4}g^{il}\left\{2\frac{\partial g_{jl}}{\partial x^k} - \frac{\partial g_{jk}}{\partial x^l}\right\}y^jy^k, \qquad (4)$$

where

$$g_{ij}\left(x^k, y^k\right) = \frac{1}{2}\frac{\partial^2 F^2}{\partial y^i \partial y^j},$$

$x^j = (t(s), r(s), \varphi(s))$ and $y^j \equiv (\dot{\xi} = \frac{dt}{ds}, \dot{r}(s), \dot{\varphi}(s))$. Further, the evolution parameter s associated with the geodesics in the configuration space with the metric parameters (2-3) will be denoted as s_w.

In fig. 1 the geodesics in the monolayer configuration space, the compression isotherms $s_w(r)$ and corresponding potentials U are shown for very low and high enough compression rates $V = 10^{-25}$ and $V = 7 \cdot 10^{-3}$, respectively. The metric function (2-3) defines the phase transition dynamics. Because of this fact the value of the domain-wall velocity, and, consequently, velocity of the billiard boundary, can be considered to equal to the velocity $\dot{r}$.

3. Numerical method and results of simulation

The movement of the probe particle in the billiard occurs along the geodesics given by the Euler-Lagrange equations (4) in the space with the metric function of the same type (2) but with fixed parameters:

$$A = 10^{-5}, \; B = 1, \; m = 1. \qquad (5)$$

The geodesics of the probe particle can be found in parametric form using an evolution parameter s_b.

The chosen parameters (5) define small deviation of the Finsler function (2) from a pseudo-Riemannian metric that is a limit one at very low compression rates $V \to 0$. On the billiard boundary the particle reflects in accordance with the formulas [19]:

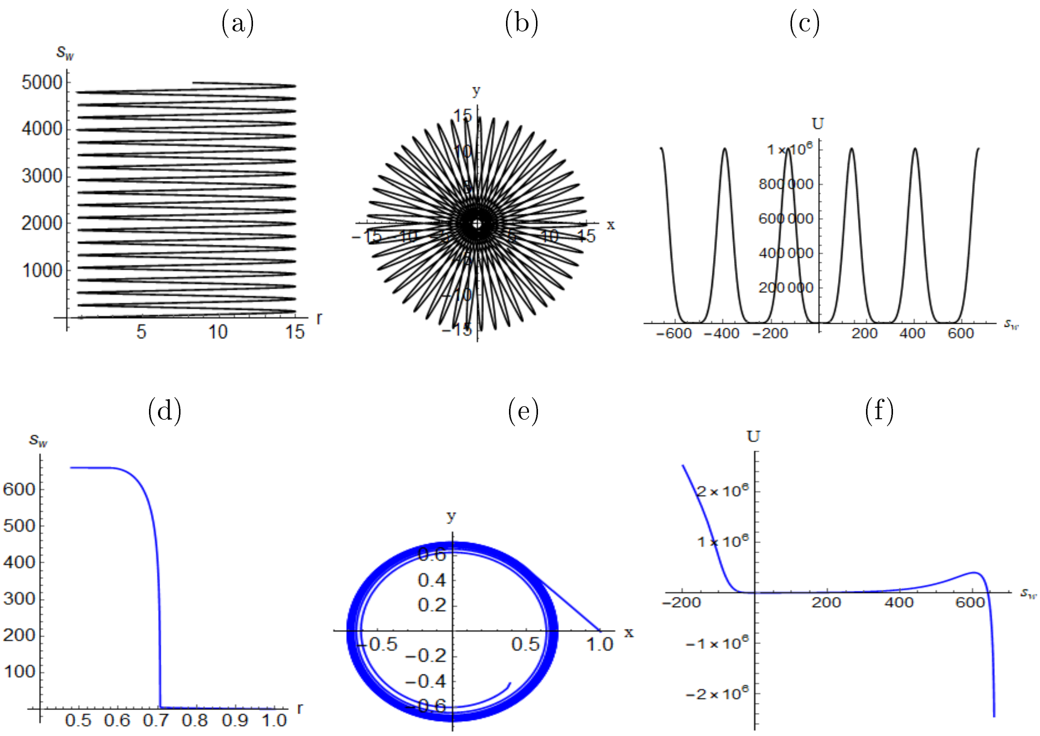

Figure 1: Compression isotherms $s_w(r)$ (a, d), geodesics (b, e) in the configuration space and potentials $U(s_w)$ (c, f) at the following model parameters: $V = 10^{-25}$ (a-c) and $V = 7 \cdot 10^{-3}$, (d-f); $p = 10^{-8}$, $m = 1$.

$$v'_{v,rel} = -\frac{v_{v,rel} - 2V_d + V_d^2 v_{v,rel}/\tilde{c}_{light}^2}{1 - V_d\left(2v_{v,rel} + V_d\right)/\tilde{c}_{light}^2}, \tag{6}$$

$$v'_{\tau,rel} = \frac{v_{\tau,rel}\left(1 - V_d^2/\tilde{c}_{light}^2\right)}{1 - V_d\left(2v_{v,rel} + V_d\right)/\tilde{c}_{light}^2}, \tag{7}$$

where $v_{v,rel}$ and $v'_{v,rel}$ are normal components of the particle velocity before and after reflection, respectively, $v_{\tau,rel}$ and $v'_{\tau,rel}$ are tangential components of the particle velocity before and after reflection. The rate of the billiard wall V_d is given by the expression

$$V_d = \left(\frac{\partial \vec{r}_w}{\partial t}\right)_R \sqrt{2}B^2\left(\frac{A}{B} + \frac{\partial r_w}{\partial t}\right)^{-1} = \left(\frac{\partial r_w}{\partial t}\right)_R \sqrt{2}\left(10^{-5} + \frac{\partial r_w}{\partial t}\right)^{-1}. \tag{8}$$

Here the velocity

$$\frac{\partial \vec{r}_w}{\partial t} = \frac{\dot{\vec{r}}_w(s_w)}{\dot{t}_w(s_w)},$$

$\dot{r}_w(s_w)$ and $\dot{t}_w(s_w)$ are the derivatives of the geodesics of the space with the metric parameters (3) over the evolution parameter s_w. The derivative is taken at the point $s_w = k \cdot s_b$, where s_b is the evolution parameter for the probe particle in the billiard at its collision with the boundary, k is a scale coefficient chosen in such a way that 500 reflections of the probe particle can be packed in the range of compression isotherm. Introducing of the scale coefficient is equivalent to scaling of the motion equations and can be used owing to scale invariance of the phase transition. $\left(\frac{\partial \vec{r}_w}{\partial t}\right)_R$ is a component of the vector $\frac{\partial \vec{r}_w}{\partial t}$ that is orthogonal to the billiard boundary.

In the case when the boundary rate has the value such that the velocity of the particle after reflection takes the positive value (is directed outwards the billiard boundary), the particle is considered as a "stocked" one: $v'_{v,rel} = 0$. On the next step the particle takes the radial component of the velocity according the formula (6).

Owing to the shape of the metric used, at the constant absolute value of the initial velocity the different initial points in the space correspond to the different microstates but to the same macrostate of a Gibbs ensemble. Because of this fact the ensemble-averaged visiting set can be considered as a distribution function at given mean energy. For this energy the entropy is defined in ordinary way and can be calculated using the Boltzmann formula $S(E) = -k_B \sum_i p_i \,\mathrm{Log}\, p_i$.

In fig. 2 the typical non-closed billiard trajectories and corresponding visiting sets are shown for the case of immovable billiard boundary. In the limiting case of very small compression rates V (at $V \to 0$) the metric function (2) degenerate into a flat Minkowski metric. Due to this fact the occupancy of the billiard by the trajectories in fig. 2b preserves the spherical symmetry. Analysis of the density of billiard trajectories in fig. 2a demonstrates that there exist circular orbits inside the billiard. With increase the rate V and, respectively, the value of parameter A the billiard occupancy is distorted from spherical symmetry, as one can see in fig. 2d. But similarly to the previous case, there exist an attractor of the billiard trajectories. The occupied region of the visiting set is significantly narrowed (fig. 2c).

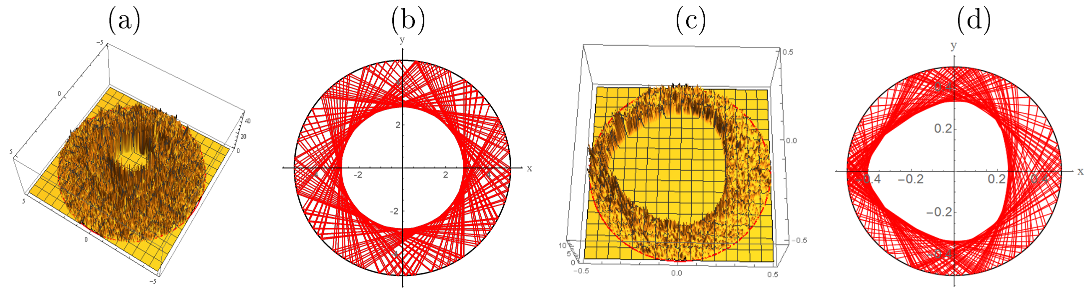

Figure 2: Visiting sets (a,c) and corresponding billiard trajectories (b,d) at negligible velocity of domain wall ($V_d = 0$) and small ($A = 10^{-25}$) (a,b) or high ($A = 10^{-5}$) (c,d) compression rates.

The results obtained for relativistic billiard model with moving boundary are shown in fig. 3. Here, the visiting sets and the billiard occupancies are represented as a sum of 9 individual trajectories that start with different initial coordinates of the probe particle but with the same absolute values of its initial velocity.

As figs. 3a,b show, at small values of the compression rate V the probability of finding of the particle with given mean energy is equal for any billiard point. It means that the configuration space is characterized by an uniform distribution function. In contrast to the billiard with immovable boundary, in this case the visiting set is radially symmetric one. Bending of the monolayer configuration space and, consequently, metric disturbance by domain-wall collisions are absent at small V.

At high compression rates V the occupied region of the visiting set is narrowed similarly to the case of immovable boundary. The bending subsets placed radially one to another appear in the visiting set at high values of V. The last indicates the wave-shape perturbation of the initially flat metric.

The growth of the new phase domain is a result of their collisions with elements of the old phase or with each other. From the considered billiard dynamics one can conclude that

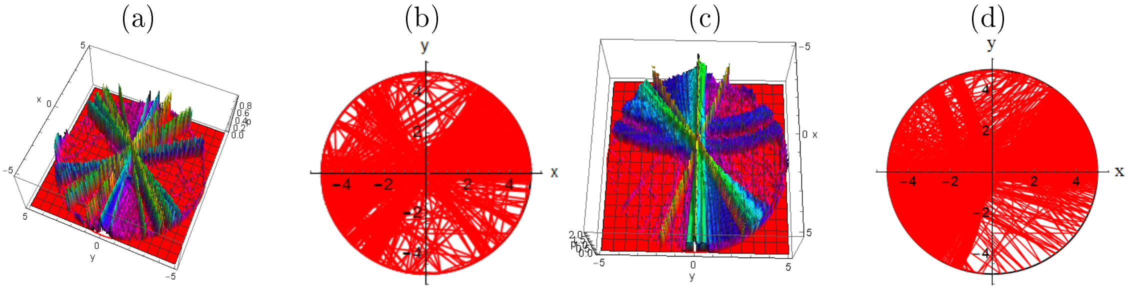

Figure 3: Visiting sets (a, c) calculated as a sum of 9 billiard trajectories (b, d) for configuration space at following model parameters: $V = 10^{-25}$, $p = 10^{-8}$ (a, b) and $V = 7 \cdot 10^{-3}$, $p = 1$ (c, d).

in the case of slowly compression the collisions take place with equal probability for any point of the domain wall. It should result in the growth of symmetrical circular domains. Appearing of the dedicated directions in the billiard model at high compression rates should reveals the separated regions of domain wall in which the probability of collisions is higher. It leads to the growth of asymmetric domains along such separated directions.

4. Conclusion

The model of two-dimensional pseudo-Finsler billiard with moving boundary and relativistic law of reflection has been constructed to describe the influence of collisions of domain walls. It has been shown that in the case of low compression rates the collisions occur equiprobably along the whole boundary of domain wall that leads to the growth of the symmetrical circular domains. The anisotropy of the configuration space at high velocities of the domain wall reveals in the distortion of visiting subsets along defined directions and results in the appearance of domains asymmetry.

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