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INVERSE STRUCTURAL STATES OF THE STOCHASTIC DEFORMATION FIELD OF FRACTAL DISLOCATION

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Исследуются новые структурные состояния фрактальной дислокации на основе теории дробного исчисления и операторов Гамильтона. В рамках статистического подхода для описания поведения стохастического поля деформации фрактальной дислокации вводятся усредненные комплексные функции. Выполнено численное моделирование поведения комплексного поля деформации на прямоугольной дискретной решетке. Показано, что для инверсных (с отрицательным фрактальным индексом) структурных состояний фрактальной дислокации существует интервал изменения этого индекса с аномальным поведением поля деформации: внутри интервала отсутствует эффективное затухание. Введенные усредненные функции позволяют выявить наличие квантовых и необычных статистических свойств поля деформации.

Ключевые слова: фрактальная дислокация, стохастическое поле деформации, численное моделирование, статистические свойства, инверсные структурные состояния

Досліджуються нові структурні стани фрактальної дислокації на основі теорії дробового обчислення й операторів Гамільтона. У рамках статистичного підходу для опису поведінки стохастичного поля деформації фрактальної дислокації вводяться усереднені комплексні функції. Виконано чисельне моделювання поведінки комплексного поля деформації на прямокутній дискретній решітці. Показано, що для інверсних (з негативним фрактальним індексом) структурних станів фрактальної дислокації існує інтервал зміни цього індексу з аномальною поведінкою поля деформації: всередині інтервалу відсутнє ефективне затухання. Введені усереднені функції дозволяють виявити наявність квантових і незвичайних статистичних властивостей поля деформації.

Ключові слова: фрактальна дислокація, стохастичне поле деформації, чисельне моделювання, статистичні властивості, інверсні структурні стани

1. Introduction

Last time many actively try to explain different experimental anomalous properties of a physical object on the basis of the definition of the fractal [1]. An adequate description of anomalous behavior of physical parameters near phase transitions, real structure of the lattice in real samples of magnets, ferroelectrics, high-temperature superconductors, amorphous alloys [2] requires a model of a nonlinear lattice with the spontaneous deformation to be further developed on the basis of qualitatively new representations of the nature of fractal and stochastic properties of the lattice. Among the real nanomaterials, active nanostructural elements are clusters, pore, quantum dots, wells, corrals, surface superlattices (see [3,4]). Active nanostructural elements can find their application in quantum nanoelectronics [5], quantum informations, quantum optics [6]. The fractal dislocation [7,8] is one of non-classical active nanostructural objects. For the theoretical descriptions of fractal objects, the theory of fractional calculations [12] has been proposed [9–11]. The fractal string model has been proposed. The equations with fractional space-time derivatives have been introduced in order to describe plastic subsystem of a fractal string. To solve the basic dynamic equation in fractional derivatives, two approaches have been suggested: reduction to a system of equations and the use of composition formulas for fractional derivative operators. The obtained results have been generalized to the solution of the Cauchy problem in the matrix form. The fractal string model was used in order to construct a model of a fractal dislocation [13–16]. The inverse structural states of fractal dislocation are investigated in this paper.

2. The model and simulations

Plasticity of materials is determined by the motion of an ensemble of dislocations. In article [13] the dynamic equations for the anisotropic plastic subsystem of a fractal medium are obtained explicitly on the basis of the fractional calculus model. For the special case of isotropic fractal medium [9–11], the original equation for the fractal string is

$$D_t^{\nu}\left(\rho_{\nu} D_t^{\nu}\Phi_{\alpha}\right) = D_z^{\alpha}\left(\mu_{\alpha} D_z^{\alpha}\Phi_{\alpha}\right), \tag{1}$$

where the function $\Phi_{\alpha}(t,z)$ depends only on the dimensionless variables of time t and coordinates z; ν, α are fractal indices of partial fractional derivatives of Riemann–Liouville D_t^{ν}, D_z^{α} on t, z, respectively; ρ_{ν} and μ_{α} are dimensionless effective parameters that are associated with the mass density and power characteristics of a fractal medium. Fractal indices ν, α have the meaning of fractal dimension along the axes Ot, Oz. If $\rho_{\nu}(z)$ and $\mu_{\alpha}(t)$ are functions of z and t, respectively, then (1) reduces to a system of equations for an unknown function $\Phi_{\alpha}(t,z)$ with varying eigenvalues $\lambda_{\alpha}(t)$, $\lambda_{\nu}(z)$:

$$D_t^{\nu} D_t^{\nu} \Phi_{\alpha} - w^2 D_z^{\alpha} D_z^{\alpha} \Phi_{\alpha} = 0, \quad w^2(t,z) = \mu_{\alpha}(t)/\rho_{\nu}(z), \tag{2}$$

$$D_z^{\alpha} \Phi_{\alpha} = \lambda_{\alpha}(t) \Phi_{\alpha}, \quad D_t^{\nu} \Phi_{\alpha} = \lambda_{\nu}(z) \Phi_{\alpha}, \quad \lambda_{\nu}^2(z) = w^2 \lambda_{\alpha}^2(t). \tag{3}$$

We will choose D_z^{α}, D_t^{ν}, I_z^{α} in the following form

$$D_z^{\alpha} \Phi_{\alpha} = \partial_z \int_{z_c}^{z} \Phi_{\alpha}(t,\xi) \left| z - \xi \right|^{-\alpha} \mathrm{d}\xi / \Gamma(1-\alpha), \tag{4}$$

$$D_z^{\nu} \Phi_{\alpha} = \partial_t \int_{t_a}^{t} \Phi_{\alpha}(\tau, z) \left| t - \tau \right|^{-\nu} \mathrm{d}\tau / \Gamma(1-\nu), \tag{5}$$

$$I_z^{\alpha} \Phi_{\alpha} = \int_{z_c}^{z} \Phi_{\alpha}(t,\xi) \left| z - \xi \right|^{\alpha-1} \mathrm{d}\xi / \Gamma(\alpha), \tag{6}$$

where ∂_z, ∂_t are the operators of the usual partial derivatives; Γ is the gamma function. When $z > \xi$, the operator D_z^{α} coincides with the operator of the left-sided $D_{z_c+}^{\alpha}$ and when $z < \xi$ it coincides with the operator of the right-sided $D_{z_c-}^{\alpha}$ that are fractional derivatives of Riemann–Liouville [12]. Using these operators allows to describe the behavior of the function Φ_{α} when passing through the value $z = z_c$.

Next, we find the functions Φ_{α} as solutions of equations (3) for the Cauchy-type problem [11] in two representations

$$\Phi_{\alpha} = h_1(t_{\alpha}, z) \left| t - t_a \right|^{\nu-1} E_{\nu,\nu}(\psi_{\nu}), \quad \psi_{\nu} = \lambda_{\nu}(z) \left| t - t_a \right|^{\nu}, \tag{7}$$

$$\Phi_{\alpha} = h_2(t, z_c) \left| z - z_c \right|^{\alpha-1} E_{\alpha,\alpha}(\psi_{\alpha}), \quad \psi_{\alpha} = \lambda_{\alpha}(t) \left| z - z_c \right|^{\alpha}, \tag{8}$$

$$h_1(t,z) = I_t^{1-\nu} \Phi_{\alpha}, \quad h_2(t,z) = I_z^{1-\alpha} \Phi_{\alpha}, \tag{9}$$

where $E_{\nu,\nu}(\psi_{\nu})$, $E_{\alpha,\alpha}(\psi_{\alpha})$ are the Mittag–Leffler functions [12].

To find the eigenvalues λ_{α} (or λ_{ν}), we use the Hamilton operator $\hat{H}$ of [8,14,15] for the energy spectrum of the fractal dislocation

$$\hat{H} = \hat{H}_0 + \hat{H}_b, \quad \hat{H}_0 = \varepsilon_2 \left(\hat{n}_1 + \hat{n}_2 \right) + \varepsilon_3 \hat{n}_3, \quad \hat{H}_b = \varepsilon_3 n_0 \hat{b}_3, \tag{10}$$

$$\hat{b}_3 = (1-\alpha) I_z^{\alpha} = \left[D_z^{1-\alpha}, \hat{z} \right], \quad n_0 = 1 - 2sn^2 \left(u_{\alpha}, k \right), \quad u_{\alpha} = u - u_0. \tag{11}$$

Here k, $u - u_0$ are the module and the argument of the elliptic sine; $\hat{n}_1$, $\hat{n}_2$, $\hat{n}_3$ are operators of occupation numbers of states of the dislocation with the dimensionless self-energy $\varepsilon_1 = \varepsilon_2$, ε_3; $\hat{z}$ is the coordinate operator. Variable u is the dimensionless displacement of the deformation field, which is related to the dimensionless stress field λ_{α} on Hooke's law $u = \lambda_{\alpha}/\lambda_0$, where λ_0 is the force parameter.

Note that the operators (10), (11) allow to describe inverse ($\alpha < 0$) states. This is due to the fact that in the theory of fractional calculus [12] for the values $\alpha \in$

[–1, 0], it is possible to have a transition from operators D_z^{α}, I_z^{α} to operators $D_z^{-(-\alpha)} = I_z^{-\alpha}$, $I_z^{-(-\alpha)} = D_z^{-\alpha}$. In regards to such a transition, the commutator from (11) retains its form. In this case, the old physical interpretation of the fractal dimension is preserved for the module |α|. Operators $\hat{H}_0$, $\hat{H}_b$ do not depend explicitly on time.

Let us consider the state of fractal dislocations at $t = t_c$. The function describing this state $\Phi(z) = \Phi_\varepsilon\Phi_{\alpha c}(z)$ depends only on z. Here Φ_ε is the eigenfunction of the operator $\hat{H}_0$ in the diagonal representation of the population numbers n_1, n_2, n_3; $\Phi_{\alpha c}(z) = \Phi_\alpha(t_c, z)$ is a function obtained from (8) at $t = t_c$. Further, we find the total energy E of fractal dislocation

$$\hat{H}\Phi = E\Phi, \quad \hat{b}_3\Phi_{\alpha c}(z) = \chi_{\alpha c}\Phi_{\alpha c}(z), \tag{12}$$

$$E = E_\varepsilon + \varepsilon_3 n_0 \chi_{\alpha c}; \quad E_\varepsilon = \varepsilon_2\left(n_1 + n_2\right) + \varepsilon_3 n_3. \tag{13}$$

From (13), (2), (12) we receive the system of the nonlinear equations for g_1, λ_{ac}

$$g_1 = (1-\alpha)/\chi_{\alpha c} = (1-\alpha)\varepsilon_3 n_0/\left(E - E_\varepsilon\right), \tag{14}$$

$$\lambda_{\alpha c}^2 = \lambda_\nu^2(z)/w^2\left(t_c, z\right) = g_1^2, \tag{15}$$

$$|g_1| = |z - z_c|^{-\alpha} E_{\alpha,\alpha}\left(\psi_{\alpha c}\right)/E_{\alpha,2\alpha}\left(\psi_{\varepsilon c}\right), \quad \psi_{\alpha c} = \lambda_{\alpha c}|z - z_c|^{\alpha}. \tag{16}$$

Modeling the behavior of the deformation field is made on a rectangular lattice with discrete sizes. $N_1 \times N_2$ Deviation of the sites of this lattice from the state with $u = 0$ is described by the operator of displacement $\hat{u}$. This operator is assigned to a rectangular matrix with the elements u_{nm}, where $n = \overline{1, N_1}$, $m = \overline{1, N_2}$. Four nonlinear model equations for $u(z, a) = \lambda_{\alpha c}/\lambda_0 = u_{\varepsilon i}(z,\alpha)$ (i = 1, 2, 3, 4) are obtained from (16)

$$2u_{\varepsilon 1} = g_1 - g_2 + g_4, \quad 2u_{\varepsilon 2} = g_1 - g_2 - g_4, \tag{17}$$

$$2u_{\varepsilon 3} = -g_1 - g_2 + g_5, \quad 2u_{\varepsilon 4} = -g_1 - g_2 - g_5, \tag{18}$$

$$g_4 = \left[\left(g_2 + g_1\right)^2 - g_3\right]^{1/2}, \quad g_5 = \left[\left(g_2 + g_1\right)^2 - g_3\right]^{1/2}. \tag{19}$$

These elements u_{nm} are found by solving nonlinear equations (17), (18) by the iteration method. An iterative procedure itself simulates a stochastic process on a rectangular discrete lattice. In general case, elements $u_{nm}(z,\alpha)$ are random complex functions of two real variables z and α, and they also depend on a number of other internal and external governing parameters. Functions g_1, g_2, g_3 for numerical simulation are in the form

$$g_1(u,\alpha) = (1-\alpha)\left(1 - 2sn^2\left(u - u_0, k\right)\right)/\left(p_0 - p_1 n - p_2 m - p_3 j\right), \tag{20}$$

$$g_2(z,\alpha) = 2^{-2\alpha} 3^{3\alpha-1/2} |z - z_c|^{-\alpha} \gamma_\alpha / \sqrt{\pi}\Gamma(\alpha + 1/2), \tag{21}$$

$$g_3(z,\alpha) = 3^{3\alpha-1/2} 2 |z - z_c|^{-2\alpha} \gamma_\alpha / \pi, \quad \gamma_\alpha = \Gamma(\alpha + 1/3)\Gamma(\alpha + 2/3), \tag{22}$$

where z_c is the critical value of the dimensionless coordinate z; p_0, p_1, p_2, p_3 are the governing parameters. A distinctive feature of the behavior of the displacement field of fractal dislocation for inverse states is the existence of an interval of fractal dimension, where the imaginary parts $u_{\varepsilon i}(z,\alpha)$ approach zero, which indicates the absence of effective damping. Within this interval, there are singular points (attractors [17]) with the values $\alpha = -1/3$ and $\alpha = -2/3$. When going through these singular points, the displacement field shows a different behavior. As an example, we give the dependency of the function $u_{\varepsilon 1}$ from the lattice nodes indices n, m for values $\alpha = -0.5$, $z_c = 2.7531$, $z = 1.753$ (Fig. 1), received by iterations method by an index m. In the modeling we have assumed that: $k = 0.5$, $j = 1$, $u_0 = 29.537$, $p_0 = 0.01$, $p_2 = p_3 = 0$; the initial condition is $u_{1,1} = 0$, $n = \overline{1;30}$, $m = \overline{1;40}$. Filling in the matrix was carried out by rows. Changing the governing parameter results in different states of fractal dislocation with stochastic behavior of the deformation field (Fig. 1).

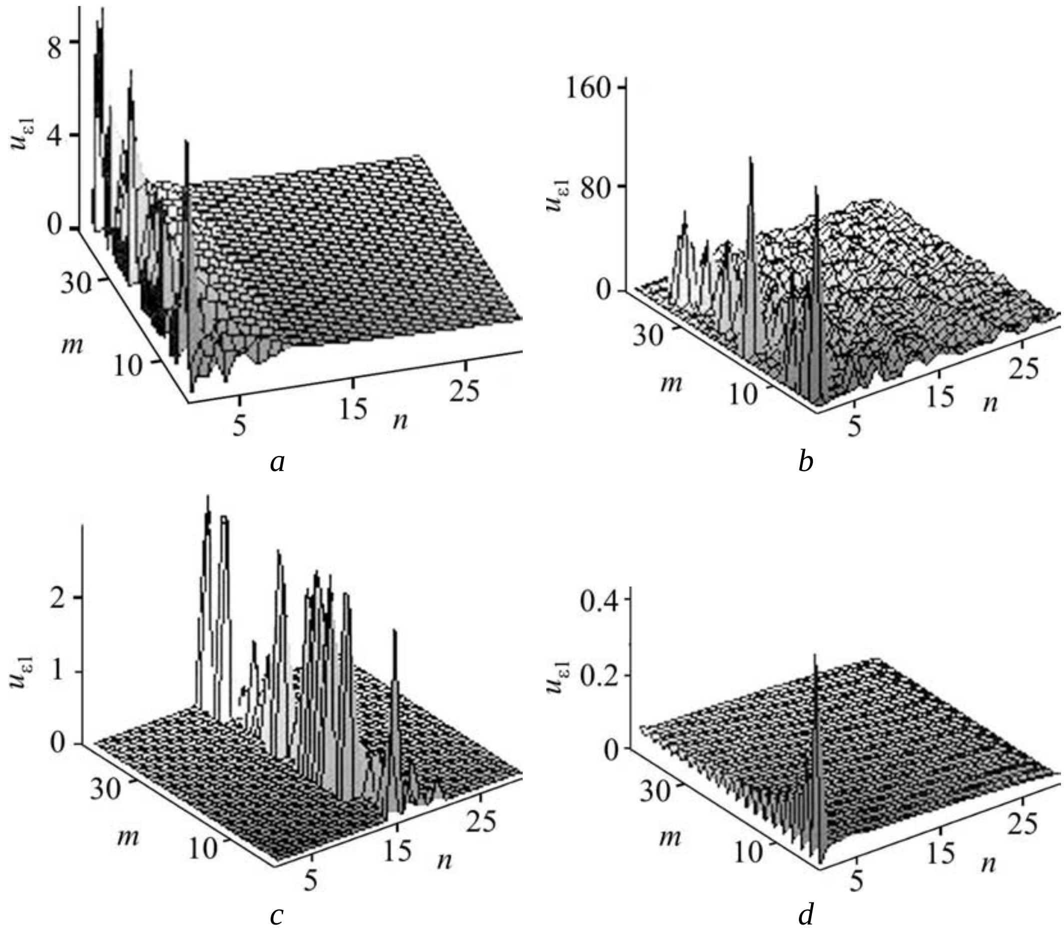

Fig. 1. The behavior of the function $u_{\varepsilon 1}$ depending on n, m for the fractal dislocation

On Fig. 1,*a*, the dislocation is located near the lower boundary ($n = 1$). The localization region of the dislocation is limited to the value $n < 13$. When $n > 13$ the surface $u_{\varepsilon 1}(n, m)$ is close to a smooth one. Plane singularities of the dislocation are located at $n_c = p_0/p_1 = 0.06579$ and go out of the lower boundary. Decrease in the parameter p_1 (Fig. 1,*b*,*c*) results in an increase in value n_c, which is accompanied by a shift of fractal dislocation parallel to the axis m. In this case, a regular deviation of the rectangular lattice nodes with $u_{\varepsilon 1} \neq 0$ starts to appear at the lower boundary, and the range of the randomization applies to all other nodes in the lattice (Fig. 1,*b*). For the lattice nodes with $n < 13$, the regular behavior is characteristic, and for $n > 13$, the stochastic behavior is observed (Fig. 1,*c*). In this case there are deviations at the boundary sites ($n = 1$) of the damping amplitude wave type. With further decrease in p_1, the plane of the singular points of the dislocation comes out of the specified region of the lattice (Fig. 1,*d*). Moreover, for all the lattice sites, the regular behavior with $u_{\varepsilon 1} \neq 0$ is characteristic. The presence of the sites, with the deviations type wave with damping amplitude along the axis m is clearly expressed at the lower boundary.

The analysis of the behavior of the deformation field in the various nodal planes $z = z_j$ is convenient to be made in terms of averaged functions M_i with the operator of the density of states $\hat{\rho}$ and matrix elements p_{nm}

$$M_i\left(z,\alpha\right) = Sp\left(\hat{\rho}\hat{u}_{\varepsilon i}\right), \quad \hat{\rho} = \hat{\xi}_{N_2}^{T}\hat{\xi}_{N_1} / N_2 N_1, \quad \sum_{m=1}^{N_2}\sum_{n=1}^{N_1}\rho_{mn} = 1, \tag{23}$$

where Sp, T are the operations of calculating the trace of square matrix, transposition; $\hat{\xi}_{N_1}$, ξ_{N_2} are the row-vectors of dimension $1 \times N_1$, $1 \times N_2$, respectively, and the elements equal to unity. The averaging is performed over the nodes of a discrete rectangular lattice (n, m), and in directions perpendicular to the plane of the lattice, the averaging is absent. This makes it possible to obtain the dependency of the averaged functions from z and identify their clearly expressed stochastic behavior for all four branches of the dimensionless displacement function $u_{\varepsilon i}$ (Fig. 2). The presence of the step-type behavior of a lattice is closely connected with the occurrence of quantum properties and quantum chaos [3] at average functions of fractal dislocation. In modeling, we assumed that $z = z_j = 0.053 + 0.1\,(j - 1)$, where $j = \overline{1;67}$. Values z were varied in the interval [0.053; 6.653] with the step $z_h = 0.1$.

When $z = z_1$ the values M_3, M_2 (Fig. 2,*a*) and M_1, M_4 (Fig. 2,*c*) are zero. Near $z = z_{28}$ the features of the global local minima and maxima type with a nonzero gap between the curves *2*, *4* (Fig. 2,*d*) and *1*, *4* (Fig. 2,*f*) are observed. The effect of mixing-up curves is observed when changing z. The behavior of the functions M (of soft mode type) at $z = z_1$ and near $z = z_{28}$ agrees with the behavior of fractal dislocation displacements (Fig. 1).

3. Conclusions

A model of fractal dislocation is constructed on the basis of the coupled system of the following equations: the dynamics for fractal strings with the operators of fractional derivatives, the Hamiltonian operator for the energy spectrum of fractal dislocation and Hooke's law, which describes the connection between stress and strain of a fractal dislocation. Within the framework of this model, the simulation of the deformation field of dislocation has been executed. For the inverse of the structural states of the fractal dislocation, the soft-mode type behavior is observed. The stochastic behavior, the change of the states of the dislocation, the absence of the effective damping and unusual quantum properties are observed near singular points (attractors).

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INVERSE STRUCTURAL STATES OF THE STOCHASTIC DEFORMATION FIELD OF FRACTAL DISLOCATION

New structural states of fractal dislocation are investigated on the basis of fractional calculation theory and Hamilton operators. In order to describe the behaviour of the stochastic deformation field of a fractal dislocation within the framework of the statistical approach, average complex functions are introduced. Numerical modelling of the complex deformation field behaviour is fulfilled on a rectangular discrete lattice. It is shown that for inverse (with a negative fractal index) states of a fractal dislocation, there is an interval of change of this index with anomalous behaviour of the deformation field: there is no effective attenuation within the interval. The introduced functions allow to educe the presence of quantum and unusual statistical properties of the deformation field.

Keywords: fractal dislocation, stochastic deformation field, numerical modeling, statistical properties, inverse structural states