Governance of Alteration of the Deformation Field of Fractal Quasi-Two-Dimensional Structures in Nanosystems

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Abstract: A model nanosystem is investigated: a sample in the form of a rectangular parallelepiped of finite size with volumetric discrete lattice. It is shown that a separate nodal plane of a model nanosystem can be in different structural states: stochastic state of the deformation field on the whole rectangular lattice; the state with the linear fractal dislocation of different orientations; quasi-two-dimensional structures of the type of fractal elliptical, hyperbolic dislocations and fractal quantum dot. Using the numerical modelling method, the behaviour of the deformation field and a possibility of the alteration of these structures is investigated. The analysis of the behavior of the averaged functions allows to determine the critical values of the governing parameters.
Keywords: fractal quasi-two-dimensional structures, nanosystem, stochastic deformation field, numerical modeling, averaged functions, alteration of the structure.

1. Introduction

Investigation of fundamental properties of nanosystems and nanomaterials of a new generation [1, 2] is actual for modern areas of science and nanotechnology. Among the real nanomaterials the active nanostructural elements are clusters, porous, quantum dots, wells, corrals, surface superlattices. The physical properties of these elements can demonstrate chaotic behavior [3]. The active nanostructural elements can find their application in the quantum nanoelectronics, quantum informations [4], quantum optics. Previously in paper [5] fractons – vibrational excitations on fractals – were introduced. Fractal dislocation [6, 7] is one of the non-classical active nanostructural objects. For the theoretical descriptions of fractal objects it has been proposed [6, 7] to use the theory of fractional calculations [8] and the concept of fractals [9]. The new structural states [10-13] of fractal dislocation were investigated on the basis of fractional calculation theory and Hamilton operators. The purpose of the paper is to research a possibility of governing the alteration of the deformation field of fractal quasi-two-dimensional structures in model nanosystems.

2. Basic nonlinear equations

A model nanosystem is investigated: a sample in the form of a rectangular parallelepiped of a finite size with volumetric discrete lattice $N_1 \times N_2 \times N_3$,

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whose nodes are given integers n, m, j ($n=\overline{1,N_1}$; $m=\overline{1,N_2}$; $j=\overline{1,N_3}$). In papers [11] the dimensionless variable displacement u of the lattice nodes is described by function

$$u=(1-\alpha)\left(1-2\,sn^2(u-u_0,\,k)\right)\Big/Q\,,\quad Q=p_{01}-p_1 n-p_2 m-p_3 j\,. \quad (1)$$

Here α is the fractal dimension of the deformation field u along the Oz-axis ($\alpha\in[0,1]$); u_0 is the constant (critical) displacement; k is the modulus of the elliptic sine; governing parameters p_{01}, p_1, p_2, p_3 do not depend on the integers n, m, j. This paper takes into account the parameters p_{01}, p_1, p_2, p_3 depending on the integers n, m, j. While modeling deformation fields of stochastic fractal quasi-two-dimensional structures, this allowed to obtain the basic non-linear equations that take into account the interaction of nodes in the plane of the discrete rectangular lattice $N_1\times N_2$. The structure of these equations is similar to the expression (1), but with a different value of the function Q. For a linear fractal dislocation the function Q has the form

$$Q=p_0-b_1\left((n-n_0)/n_c\right)-b_2\left((m-m_0)/m_c\right); \quad (2)$$

$$b_1=\cos(\pi/2+\varphi(j))\,;\quad b_2=\cos\varphi(j)\,. \quad (3)$$

For other fractal quasi-two-dimensional structures the function Q has the form

$$Q=p_0-b_1\left((n-n_0)/n_c\right)^2-b_2\left((m-m_0)/m_c\right)^2, \quad (4)$$

where for the elliptic dislocation and fractal quantum dot

$$b_1=b_2=\cos\varphi(j) \quad (5)$$

and in the case of fractal hyperbolic dislocation

$$b_1=\cos\varphi(j)\,;\quad b_2=\cos(\pi+\varphi(j))\,. \quad (6)$$

Now here the governing parameters are $p_0, n_0, n_c, m_0, m_c, \varphi(j)$. Varying these parameters both a structural state of the self-fractal dislocation and the type of dislocation (for example, the transition from fractal elliptical dislocation to fractal quantum dot) can be governed. In general case the governing parameters can be changed from one node plane to another, which may be connected not only with external governance (for example, when a parameter p_0 is changed), but also with internal governance (the process of self-organization of structures when $\varphi(j)$ is changed). To investigate the behavior of the stochastic deformation field of fractal quasi-two-dimensional structure in terms of the statistical approach, averaged functions are introduced [11]. The necessity of averaging is connected with the fact that the elements of the lattice nodes displacement matrix are in general case random real functions. The average is taken only on nodes in the plane of the discrete rectangular lattice $N_1\times N_2$. For this the operators fields of displacement $\hat{u}$ and density of states $\hat{\rho}$ are introduced. These operators are coincided to the matrix with the elements of u_{nm}; $\rho_{mn} = 1/N_2 N_1$. Rectangular matrices $\hat{u}$ and $\hat{\rho}$ have the dimensions of $N_1 \times N_2$; $N_2 \times N_1$, respectively. For a homogeneous distribution the operator $\hat{\rho}$ is given by

$$\hat{\rho} = \hat{\xi}_{N2}^T \hat{\xi}_{N1} / N_2 N_1, \tag{7}$$

where «T» denotes transposition; $\hat{\xi}_{N1}$, $\hat{\xi}_{N2}$ are row-vectors with elements equal to one. The averaged function M has the form [11]

$$M = Sp(\hat{\rho}\hat{u}) = M' + i M''; \quad M' = \operatorname{Re} M; \quad M'' = \operatorname{Im} M. \tag{8}$$

Here Sp is an operation of calculating the trace of a square matrix; Re, Im represent an allocation of real and imaginary parts of the complex function M; i is an imaginary unit. Averaged function M depends on the governing parameters $p_0(j)$, $\varphi(j)$. In general case $M = M(j)$ is a random function, as an average over the index j is not made. This means that there are some critical values $p_0(j)$, $\varphi(j)$, during the transition through which the behavior of function M can vary from regular to stochastic. Therefore there is a problem of finding the critical values of these governing parameters.

3. Numerical simulation and the analysis of results

Solution of the nonlinear equation (1) with the value of function Q in the form (3) is constructed by the iteration method [11] for fixed values $\alpha = 0,5$; $k = 0,5$; $u_0 = 29,537$. The iterative procedure on the index m simulates a stochastic process on a rectangular discrete lattice with a size $N_1 \times N_2 = 30 \times 40$. The initial parameters were the following: $n_0 = 14,3267$; $n_c = 9,4793$; $m_0 = 19,1471$; $m_c = 14,7295$. In the simulation it was assumed that $\varphi(j) = (j-1)\pi/10$. A separate nodal plane of a model nanosystem can be in different structural states: the state with the linear fractal dislocation of different orientations (Fig. 1); stochastic state of the deformation field on the whole rectangular lattice (Fig. 2. b, Fig. 3. b); quasi-two-dimensional structures of the type of fractal elliptical (Fig. 2. a), hyperbolic dislocations (Fig. 3. a. c) and fractal quantum dot (Fig. 2. c). Governance of alteration (Fig. 1-Fig. 3) of the deformation field is achieved by changing the internal parameters b_1, b_2. At the same time the external parameter $p_0 = 0.1453$ has been fixed and is chosen from the field of stochastic behavior of the averaged function M (Fig. 4-Fig. 6). Rotation of a linear dislocation (Fig. 1) is achieved by governing the internal parameters b_1, b_2 (3) by changing the angle $\varphi(j)$. At rotation there is a change of the structural state of the dislocation and substructures appear, which is related to the influence of the stochastic iteration process along the axis Om. If $\cos\varphi(j) > 0$ the quasi-two-dimensional structure (4), (5) is a structure of the type of fractal elliptical dislocation, for which the location of the singular points is typical for real ellipse. If $\cos\varphi(j) < 0$ the quasi-two-dimensional structure is a structure of the type of the fractal quantum dot [12], for which the location of the singular points is typical for an imaginary ellipse. Fig. 2 show the transition from the elliptic dislocation to the quantum dot through the stochastic state of the whole lattice.

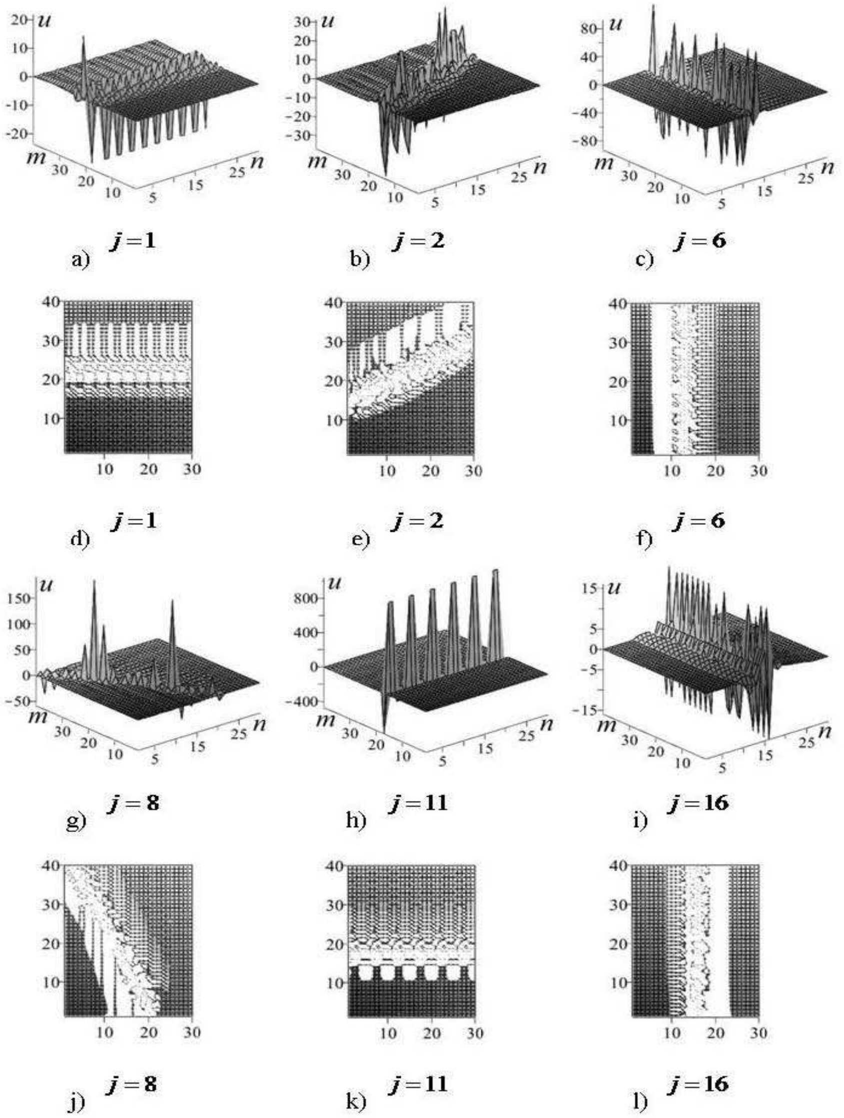

Fig. 1. The behavior of functions u (a,b,c,g,h,i) and their cuts (d,e,f,j,k,l) at $u \in [-0.5, 0.5]$ (top view) depending on the lattice index n and m for linear fractal dislocation

This transition is realized when governing the internal parameters of b_1, b_2 (5) by changing the angle $\varphi(j)$. At the same time a reorientation of the peaks, a change of the substructure, an expansion (at $j \in [1,5]$) and a restriction (at $j \in [17,21]$) of the area of the elliptical dislocation; a restriction (at $j \in [7,11]$) and an expansion (at $j \in [12,15]$) of the area of the quantum dot are observed.

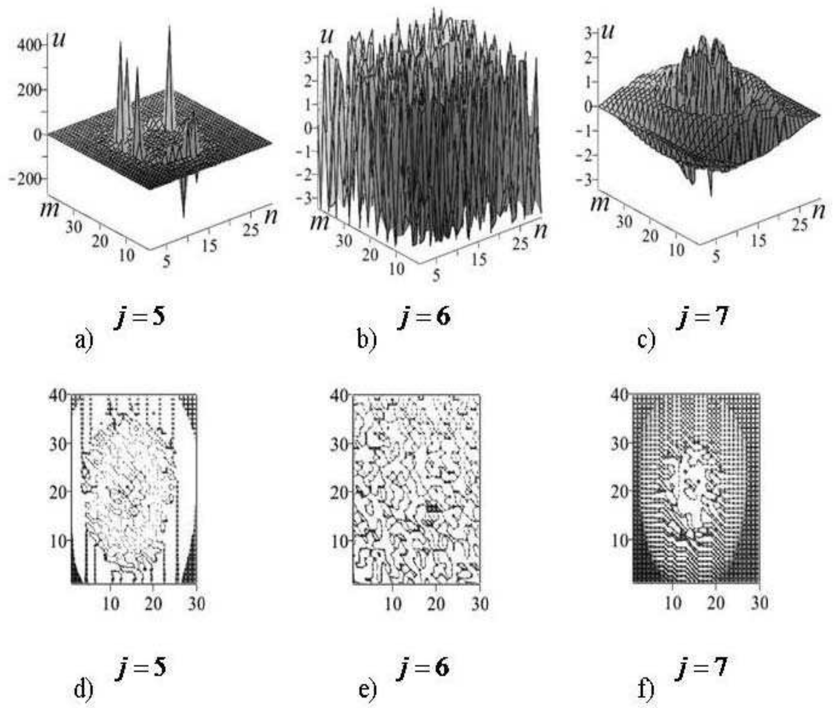

Fig. 2. The transition from the elliptic dislocation to the quantum dot. The behavior of the functions u (a,b,c) and their cuts (d,e,f) at $u \in [-0.5, 0.5]$ (top view) depending on the lattice index n and m

The reorientation of the branches of the fractal hyperbolic dislocation through the stochastic state of the whole lattice is achieved by governing the internal parameters b_1, b_2 from (6) by changing the angle $\varphi(j)$ (Fig. 3). Strongly pronounced stochastic behavior of the deformation field and the substructure can be observed for the region between the branches of the hyperbolic dislocation. The analysis of the behavior of the averaged functions allows to determine the critical values of the governing parameters. In our case, the parameter p_0 is a parameter of the external governance, averaged function M is a real random function. The behavior of function M for the fractal elliptical dislocation ($p_0 > 0$, $b_1 = b_2 = 1$) is shown in Fig. 4. In the interval of $p_0 \in [0;5]$ a base peak (Fig. 4. a) and a stochastic behavior with smaller amplitudes (Fig. 4. b) are observed. The presence of several features (such as local resonance dispersion) allows us to determine the critical values of p_0, during the transition through which the stochastic behavior of M is changed to a regular one(Fig. 4. c). These features allow us to study the mechanism of alteration of fractal quasi-two-dimensional structures of the type of elliptical dislocation. With a further increase in p_0 function M is regular and asymptotically approach to zero from negative values.

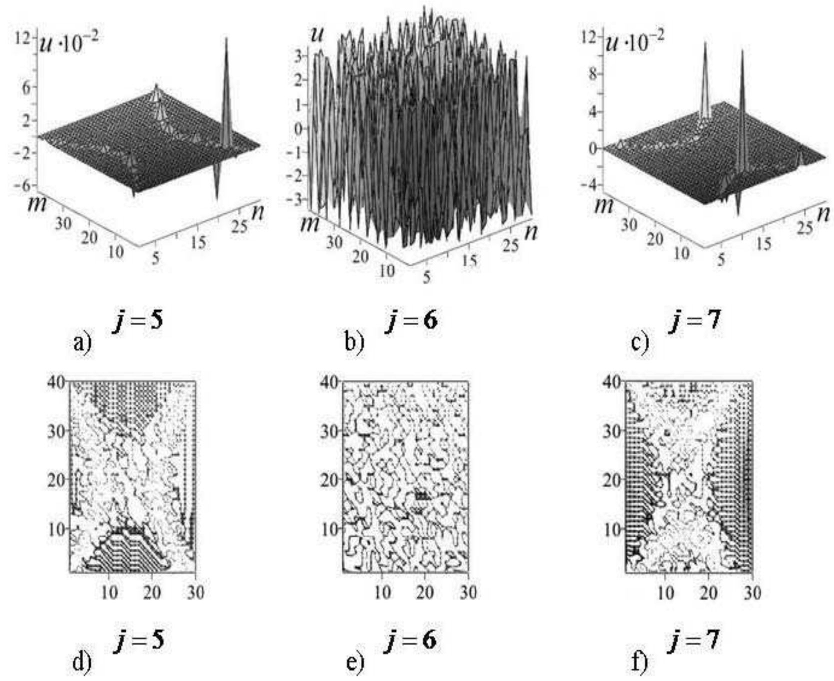

Fig. 3. The reorientation of the branches of the hyperbolic dislocation through the stochastic state. The behavior of the functions u (a,b,c) and their cuts (d,e,f) at $u \in [-0.5, 0.5]$ (top view) depending on the lattice index n and m

The behavior of M for the fractal quantum dot ($p_0 < 0$, $b_1 = b_2 = 1$) is shown in Fig. 5. When changing p_0 the regular behavior of function M (Fig. 5. a) goes into pronounced stochastic (Fig. 5. b). The presence of such features as inflection points, local maxima and minima allows to determine the critical values of the parameter p_0 (Fig. 5. c). The behavior of the function M of the parameter p_0 at $b_1 = -1$, $b_2 = 1$ ($j = 11$) for the fractal hyperbolic dislocation (4), (6) is shown in Fig. 6. By changing p_0 a base peak and two additional peaks (Fig. 6. a) are observed, as well as a pronounced stochastic behavior with smaller amplitudes (Fig. 6. b). The features of the function behavior are given by a type of local inflection points, maxima and minima (as in the quantum dot of Fig. 5. c). This allows to determine the critical value of the parameter p_0, across which the regular behavior of the function M changes to stochastic (Fig. 6. c).

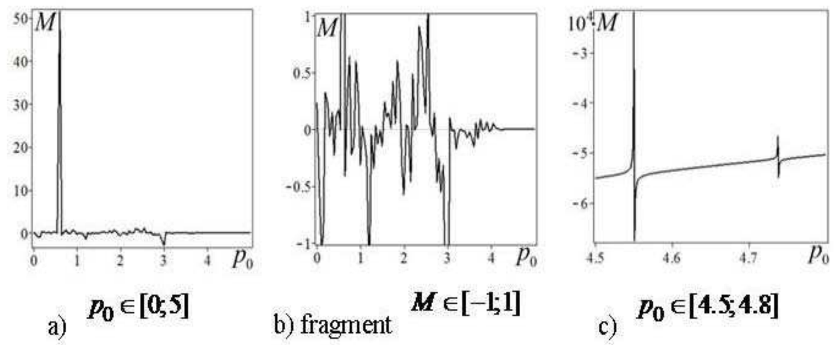

Fig. 4. The behavior of M of p_0 for the elliptic dislocation at $j = 1$

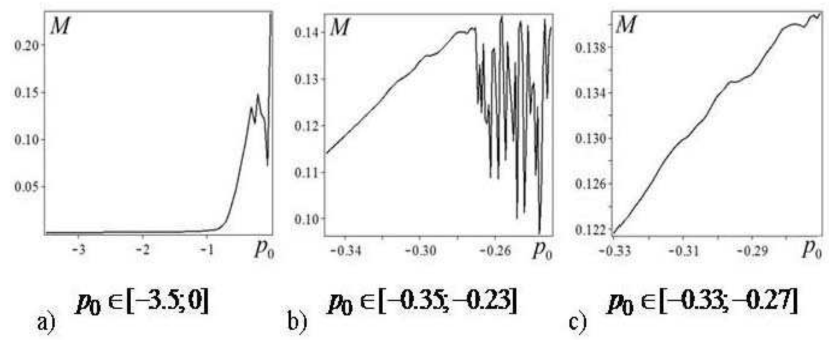

Fig. 5. The behavior of M of p_0 for the fractal quantum dot at $j = 1$

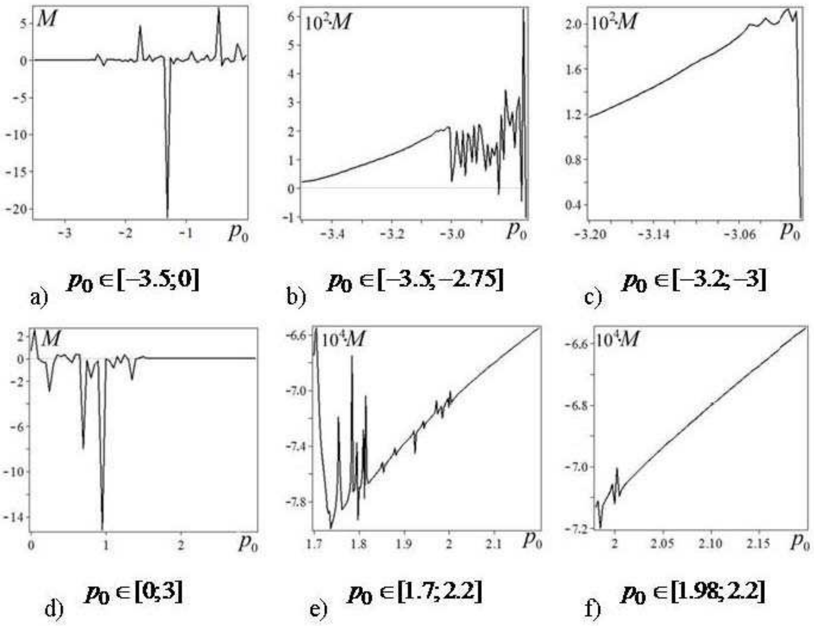

Fig. 6. The behavior of M of p_0 for the hyperbolic dislocation at $j = 11$

By changing the sign of p_0 (Fig. 6. d) there is a change in the orientation of the branches of the fractal hyperbolic dislocation. In this case the features of M have the form of a resonance dispersion type (Fig. 6. e) against the background of the step (Fig. 6. f). This allows to determine the critical value of the parameter p_0, across which the stochastic behavior of M changes to regular.

4. Conclusions

In order to describe stochastic deformation fields of fractal quasi-two-dimensional structures the basic non-linear equations taking into account the interaction of nodes in the plane of the discrete rectangular lattice were obtained. The alteration of the deformation field of fractal quasi-two-dimensional structures is achieved by changing internal and external governing parameters. It is shown that in this case both the structural state of the self-structure and the type of structure vary. The behavior of the averaged functions when changing the governing parameters correlates with the behavior of the deformation field and is related to the mechanisms of alteration of fractal quasi-two-dimensional structures.

References

1. A. Castro Neto, F. Guinea, N. Peres, K. Novoselov, A. Geim. The electronic properties of graphene. *Rev. Mod. Phys.* **81**: 109-162, 2009.
2. L. Tarruell, D. Greif, T. Uehlinger, G. Jotzu, T. Esslinger. Creating, moving and merging Dirac points with a Fermi gas in a tunable honeycomb lattice. *Nature* **483,** 7389: 302-305, 2012.
3. H.-J. Stockmann. *Quantum Chaos.An Introduction*. Cambridge Univers. Press, 1999.
4. M.A Nielsen, I.L. Chuang. *Quantum Computation and Quantum Information.* Cambridge: Cambridge Univ. Press, 2000.
5. S. Alexander, O. Entin-Wohlman, R. Orbach. Relaxation and nonradiative decay in disordered systems. I. One-fracton emission. *Phys. Rev. B.* **32,** 10: 6447-6455, 1985.
6. V.S. Abramov. Fractal dislocation as one of non-classical structural objects in the nano-dimensional systems. *Metallofiz. i Noveishie Tekhnologii*. **33,** 2: 247-251, 2011.
7. O.P. Abramova, S.V. Abramov. Alteration of the structure of the stochastic dislocation deformation field under the change of governing parameters. *Metallofiz. i Noveishie Tekhnologii.* **33,** 4: 519-524, 2011.
8. S.G. Samko, A. Kilbas, O. Marichev. Fractional Integrals and Derivatives. Theory and Applications. Gordon and Breach Sci. Publ., New York et alibi, 1990.
9. B.B. Mandelbrot. *The Fractal Geometry of Nature.* Freeman, New York, 1982.
10. V.S. Abramov. Behavior of the deformation field of fractal dislocation in the presence of bifurcftions. *Bul. of Donetsk Nat. Univers.* Ser. **A,** 2: 23-29, 2011.
11. O.P. Abramova, S.V. Abramov. Deterministic and stochastic governance of the alteration of the fractal dislocation structure. *Bul. of Donetsk Nat. Univers.* Ser. **A,** 2: 30-35, 2011.
12. V.S. Abramov. Inverse structural states of the deformation field of a fractal quantum dot. *Book of Abstracts CHAOS 2012 «5th Chaotic Modeling and Simulation International Conference», 12-15 June 2012 Athens, Greece.* p. 11-12, Greece, 2012.
13. O.P. Abramova, S.V. Abramov. Governing the behaviour of the deformation fields of fractal quasi-two-dimensional structures. *Book of Abstracts CHAOS 2012 «5th Chaotic Modeling and Simulation International Conference», 12-15 June 2012 Athens, Greece.* p. 12-13, Greece, 2012.