Chaotic Modeling and Simulation (CMSIM) 3 : 357-365, 2013

Correlation Relations and Statistical Properties of the Deformation Field of Fractal Dislocation in a Model Nanosystem

Valeriy S. Abramov

Donetsk Institute for Physics and Engineering named after A.A. Galkin,
National Academy of Sciences of Ukraine, Ukraine
E-mail: vsabramov@mail.ru

Abstract: A model sample of a finite nanosize with the volumetric lattice in the form of a rectangular parallelepiped is considered. On the basis of the previously proposed one-point model, a two-point model is constructed, which uses the theory of fractional calculus and the concept of fractal. The features of the behavior of the deformation field of fractal dislocation and possible correlation connections are investigated. It is shown that complex correlation connections have negative, positive and sign changing correlation coefficients. The strongly pronounced stochastic behaviour of amplitudes and phases of average functions is established. The change of the statistics from Fermi-Dirac type to the statistics of Boze-Einstein type for separate internal nodal planes is shown by the method of numerical modeling.
Keywords: fractal dislocation, nanosystem, stochastic deformation field, numerical modeling, distribution functions, correlation connections.

1. Introduction

For experimental studies of the physical properties of individual atoms (electrons, photons) and the quantum measurement it is necessary to create special traps: nanosystem - trapped particles (or group of particles) in a trap. These traps can be useful for realization of optical quantum computation with quantum information processing, measurement in quantum optics [1]. In his Nobel lecture in Physics in 1989 W. Paul [2] considered electromagnetic traps for charged and neutral particles. For the observation of Bose-Einstein condensation phenomenon [3] the magnetic traps were used. Serge Haroche and David Wineland, 2012 Nobel laureates in Physics, proposed experimental methods that made it real to measure individual quantum systems and govern them [4, 5]. The experimental studies of the features of the statistical properties of individual quantum systems in neutron spin measurements [6], with the observation of Bose-Einstein condensation [7] showed the presence of correlations in the measured values. Near singular points (Dirac points) Dirac fermions in molecular graphene show quantum and statistical features of behavior [8].

Received: 2 April 2013 / Accepted: 7 July 2013

ISSN 2241-0503

Fractal dislocation is one of the structural objects in nanostructured materials [9, 10]. The core of a linear dislocation is a set of singular points. The deformation field of fractal dislocation has unusual quantum and statistical properties [11 - 13] and shows the presence of quantum chaos [14]. Earlier a one-point model was used to describe the structural states of the deformation field of fractal dislocation [10, 12] (fractal dimension was an effective coordinate). In this model, the elements of the displacement of the lattice nodes are real random functions and were determined without the effect of bifurcation of solutions of a nonlinear equation. However, consideration of the effect of bifurcation of solutions [11] leads to the four branches of the lattice nodes displacement function. Elements of the lattice nodes displacement matrix become complex random functions. In order to describe possible correlation effects and statistical properties of the deformation field of fractal dislocation of pure structural states a two-point model was proposed [15] in which the theory of fractional calculus [16] and the concept of fractal [17] are used. It is necessary to investigate the mixed states, the description of which requires introducing the density of states and accounting for the distribution of this density of states on nodes of the volumetric lattice.
The purpose of this paper is to generalize the two-point model to the case of mixed state and investigate correlation connections and the statistical properties of the deformation field of fractal dislocation in the model nanosystem.

2. Description of mixed states in the two-point model

A model nanosystem [15] is considered: a sample in the form of a rectangular parallelepiped of finite size with volumetric discrete lattice $N_1 \times N_2 \times N_3$. Deviations of the lattice nodes from the state of equilibrium in a separate plane $N_1 \times N_2$ for two different points of $z_1(j)$ and $z_2(j)$ are described by non-hermitian displacements operators $\hat{u}(z_1)$ and $\hat{u}(z_2)$, corresponding to the rectangular matrix with dimensions $N_1 \times N_2$, $j \in [1, N_3]$.
For the description of mixed states the effective composite operators of displacements for the states $p = 1, 2, \ldots 8$ are introduced, respectively,

$$\hat{u}_1 = \hat{\rho}_{12}\hat{u}^+(z_1); \; \hat{u}_3 = \hat{\rho}_{12}\hat{u}^+(z_2); \; \hat{u}_5 = \hat{u}(z_1)\hat{\rho}_{12}^T; \; \hat{u}_7 = \hat{u}(z_2)\hat{\rho}_{12}^T; \quad (1)$$

$$\hat{u}_2 = \hat{\rho}_{21}\hat{u}(z_1); \; \hat{u}_4 = \hat{\rho}_{21}\hat{u}(z_2); \; \hat{u}_6 = \hat{u}^+(z_1)\hat{\rho}_{21}^T; \; \hat{u}_8 = \hat{u}^+(z_2)\hat{\rho}_{21}^T. \quad (2)$$

Here the symbols «+» and «T» mean the operation of hermitian conjugation and transposition. The square matrices with sizes $N_1 \times N_1$ for $p = 1, 3, 5, 7$ and $N_2 \times N_2$ for $p = 2, 4, 6, 8$ correspond to the introduced operators $\hat{u}_p$; so that $\hat{u}_5 = \hat{u}_1^+$, $\hat{u}_7 = \hat{u}_3^+$, $\hat{u}_6 = \hat{u}_2^+$, $\hat{u}_8 = \hat{u}_4^+$. The density state operators $\hat{\rho}_{12}, \hat{\rho}_{12}^T$, $\hat{\rho}_{21}, \hat{\rho}_{21}^T$ are represented by

$$\hat{\rho}_{12} = \hat{\xi}_{N1}^T \hat{\xi}_{N2} / N_1 N_2; \; \hat{\rho}_{12}^T = \hat{\xi}_{N2}^T \hat{\xi}_{N1} / N_1 N_2; \; \hat{\rho}_{21} = \hat{\rho}_{12}^T; \hat{\rho}_{21}^T = \hat{\rho}_{12}, \quad (3)$$

where $\hat{\xi}_{N1}$, $\hat{\xi}_{N2}$ are row-vectors of dimensions $1\times N_1$, $1\times N_2$, with elements equal to one. The rectangular matrices $\hat{\rho}_{12}$, $\hat{\rho}_{21}$ have dimensions $N_1\times N_2$, $N_2\times N_1$. For the operators in (3) the normalization conditions are fulfilled

$$\hat{\xi}_{N1}\hat{\rho}_{12}\hat{\xi}_{N2}^T=1;\qquad \hat{\xi}_{N2}\hat{\rho}_{21}\hat{\xi}_{N1}^T=1. \tag{4}$$

Having performed an averaging over the index nodes n,m by calculating trace Sp of square matrices (1), (2), the averaged functions u_p, $|u_p|$, $tg\varphi_p$ for states with $p=1,2,...8$ are obtained

$$u_p=Sp\hat{u}_p=u'_p+iu''_p=|u_p|\exp(i\varphi_p);\ \ u_p^*=Sp\hat{u}_p^+;\ \ tg\varphi_p=u''_p/u'_p, \tag{5}$$

where $u'_p=\mathrm{Re}\,u_p$, $u''_p=\mathrm{Im}\,u_p$; the symbol «$*$» means the operation of complex conjugation; $|u_p|$, φ_p are a module, a phase of the complex averaged functions u_p. Here the averaging across an index j is not made.

Then we find the correlation function of the first order. For $p,q=1,3,5,7$ we obtain

$$K_{pq}=S_{pq}-H_{pq}=K'_{pq}+iK''_{pq}=|K_{pq}|\exp(i\theta_{pq});$$

$$S_{pq}=Sp\hat{S}_{pq}=S'_{pq}+iS''_{pq}=|S_{pq}|\exp(i\psi_{pq});\ \hat{S}_{pq}=\hat{u}_p\hat{u}_q^+;\ \hat{S}_{pq}^+\neq\hat{S}_{pq};$$

$$H_{pq}=(Sp\hat{u}_p)(Sp\hat{u}_q^+)=u_pu_q^*=H'_{pq}+iH''_{pq}=|H_{pq}|\exp(i\delta_{pq});$$

$$|H_{pq}|=|u_p|\cdot|u_q|;\quad \delta_{pq}=\varphi_p-\varphi_q. \tag{6}$$

In the case $p,q=2,4,6,8$ we obtain

$$C_{pq}=A_{pq}-B_{pq}=C'_{pq}+iC''_{pq}=|C_{pq}|\exp(i\beta_{pq});$$

$$A_{pq}=Sp\hat{A}_{pq}=A'_{pq}+iA''_{pq}=|A_{pq}|\exp(i\chi_{pq});\ \hat{A}_{pq}=\hat{u}_p\hat{u}_q^+;\ \hat{A}_{pq}^+\neq\hat{A}_{pq};$$

$$B_{pq}=(Sp\hat{u}_p)(Sp\hat{u}_q^+)=B'_{pq}+iB''_{pq}=|B_{pq}|\exp(i\gamma_{pq});$$

$$|B_{pq}|=|u_p|\cdot|u_q|;\quad \gamma_{pq}=\varphi_p-\varphi_q. \tag{7}$$

From (6) at $p=q$ we have $\delta_{pp}=0$, $H_{pp}=|H_{pp}|=|u_p|^2$; operators $\hat{S}_{pp}=\hat{S}_{pp}^+$ are hermitian, $S''_{pp}=0$, $S_{pp}=S'_{pp}$ and

$$K_{pp}=S'_{pp}-|H_{pp}|=|K_{pp}|\exp(i\theta_{pp}). \tag{8}$$

From (8) it follows that $\theta_{pp}=\pi k$, where $k=0,\pm1,\pm2,..$ and autocorrelation function can be either positive ($k=0,\pm2,\pm4,..$) or negative ($k=\pm1,\pm3,..$). From (7) at $p=q$ we obtain $\gamma_{pp}=0$, $B_{pp}=|B_{pp}|=|u_p|^2$; then operators

$\hat{A}_{pp} = \hat{A}^{+}_{pp}$ are hermitian, $A''_{pp} = 0$, $A_{pp} = A'_{pp}$ and

$$C_{pp} = A'_{pp} - |B_{pp}| = |C_{pp}| \exp(i\beta_{pp}). \tag{9}$$

From (9) it follows that $\beta_{pp} = \pi l$, where $l = 0, \pm 1, \pm 2, ..$ and autocorrelation function can be either positive ($l = 0, \pm 2, \pm 4, ..$) or negative ($l = \pm 1, \pm 3, ..$). Having done the normalization of the above functions, we obtain the distribution function of mixed states of Bose-Einstein type and Fermi-Dirac type for $p = 1,3,5,7$ in form

$$f'_{pp} - f_{pp} = 1; \quad f'_{pp} = S_{pp} / H_{pp}; \quad f_{pp} = K_{pp} / H_{pp}; \tag{10}$$

$$F'_{pp} + F_{pp} = 1; \quad F_{pp} = H_{pp} / S_{pp}; \quad F'_{pp} = K_{pp} / S_{pp}, \tag{11}$$

and for $p = 2,4,6,8$ in form

$$f'_{pp} - f_{pp} = 1; \quad f'_{pp} = A_{pp} / B_{pp}; \quad f_{pp} = C_{pp} / B_{pp}; \tag{12}$$

$$F'_{pp} + F_{pp} = 1; \quad F_{pp} = B_{pp} / A_{pp}; \quad F'_{pp} = C_{pp} / A_{pp}. \tag{13}$$

By numerical simulation it will be shown that for mixed states all autocorrelation functions $K_{pp}(j), C_{pp}(j)$ are positive in the interval $j \in [1; N_3]$. Earlier in [15] it was shown that for pure states similar autocorrelation functions are negative.

At $p \neq q$ from (6), (7) it follows that the functions K_{pq}, C_{pq} are complex. For some values p, q these functions have a sense of cross-correlated functions (for a pair of different points z_1, z_2). In this case, to investigate the correlations it is necessary to introduce second-order correlation functions. For $p, q = 1,3,5,7$ we have

$$G_{pq} = V_{pq} - W_{pq}; \quad V_{pq} = Sp\hat{V}_{pq}; \quad \hat{V}_{pq} = \hat{S}_{pq}\hat{S}^{+}_{pq}; \quad \hat{V}^{+}_{pq} = \hat{V}_{pq};$$
$$W_{pq} = (Sp\hat{S}_{pq})(Sp\hat{S}^{+}_{pq}) = S_{pq}S^{*}_{pq} = |S_{pq}|^2. \tag{14}$$

Using (6), we find a representation for

$$|S_{pq}|^2 = (|K_{pq}| - |u_p| \cdot |u_q|)^2 + 2|u_p| \cdot |u_q| \cdot |K_{pq}|(1 + \cos\Phi_{pq}), \tag{15}$$

where $\Phi_{pq} = \delta_{pq} - \theta_{pq}$. For $p, q = 2,4,6,8$ we obtain

$$g_{pq} = v_{pq} - w_{pq}; \quad v_{pq} = Sp\hat{v}_{pq}; \quad \hat{v}_{pq} = \hat{A}_{pq}\hat{A}^{+}_{pq}; \quad \hat{v}^{+}_{pq} = \hat{v}_{pq};$$
$$w_{pq} = (Sp\hat{A}_{pq})(Sp\hat{A}^{+}_{pq}) = A_{pq}A^{*}_{pq} = |A_{pq}|^2. \tag{16}$$

Using (7), we find a representation for

$$|A_{pq}|^2 = (|C_{pq}| - |u_p| \cdot |u_q|)^2 + 2|u_p| \cdot |u_q| \cdot |C_{pq}|(1 + \cos\Psi_{pq}), \tag{17}$$

where $\Psi_{pq} = \gamma_{pq} - \beta_{pq}$. At some points $j \in [1; N_3]$ changes sign at second order correlation functions $G_{pq}(j), g_{pq}(j)$ from the expressions (14) - (17) which confirms the presence of a mixed statistics.
When describing pure states [15] of the deformation field of fractal dislocation in the two-point model, the following operators and functions were introduced

$$\hat{M}_7 = \hat{u}(z_2)\,\hat{u}^+(z_1); \quad \hat{M}_8 = \hat{u}^+(z_1)\hat{u}(z_2)\ ; \quad \hat{S}_r = \hat{M}_r \hat{M}_r^+;$$

$$S_r = Sp\hat{S}_r; \qquad H_r = (Sp\hat{M}_r)(Sp\hat{M}_r^+); \qquad K_r = S_r - H_r;$$

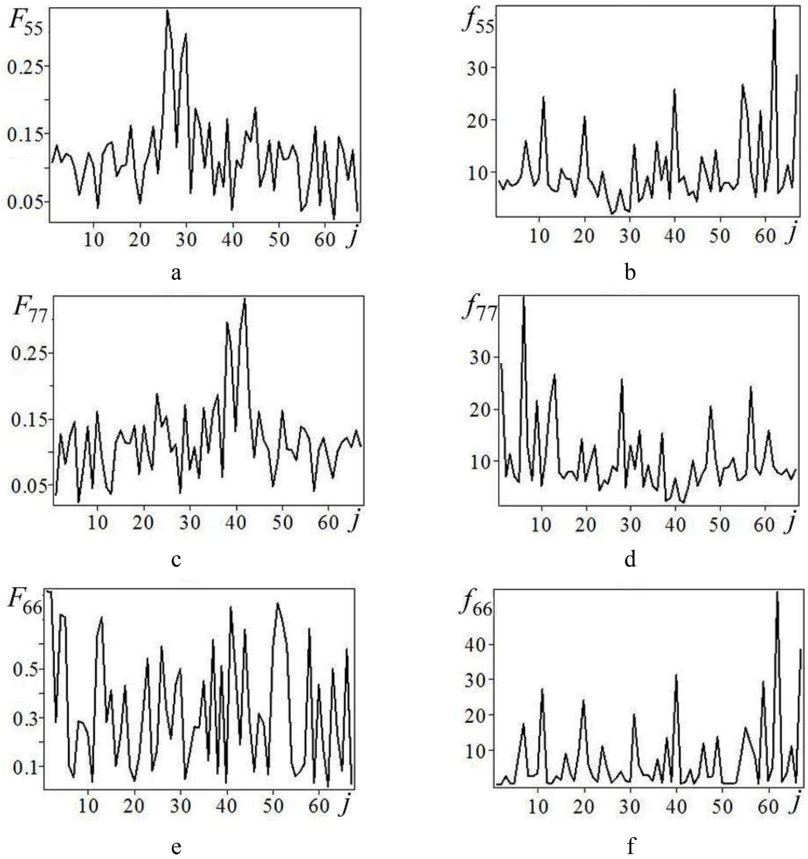
$$f_r' - f_r = 1; \quad f_r = -K_r / S_r; \quad f_r' = H_r / S_r; \quad r = 7{,}8\,. \tag{18}$$

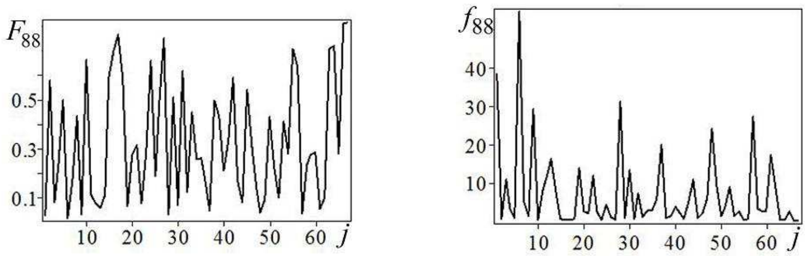
Correlation functions K_r are sign changing within the interval $j \in [1; N_3]$ and describe the states with mixed statistics.

3. Numerical simulation and the analysis of results

The original rectangular matrix displacement $\hat{u}(z_1)$ and $\hat{u}(z_2)$ with elements $u_{nm}(z_1) = u_{\varepsilon 1}(z_1)$, $u_{nm}(z_2) = u_{\varepsilon 1}(z_2)$ in bulk lattice $N_1 \times N_2 \times N_3 = 30 \times 40 \times 67$ were obtained by the method of iterations on an index m for the first branch of the dimensionless complex function displacement $u(z) = u_{\varepsilon 1}(z)$ by the formulas in [15] under the same input parameters and initial conditions. In the calculations it should be: $z_1 = 0.053 + 0.1(j-1)$; $z_2 = 6.653 - 0.1(j-1)$, which corresponds to the forward and backward waves of displacements $u_{nm}(z_1)$, $u_{nm}(z_2)$; $n = \overline{1,30}$; $m = \overline{1,40}$; $j = \overline{1,67}$. The choice of the model parameters determines the state of a discrete rectangular sublattice $N_1 \times N_2$ with fractal dislocation, localized within this region parallel to the axis Om.
The analysis of the results of the numerical simulation for the mixed states (Fig. 1) shows that all of the first-order correlation functions K_{pp} are positively defined on the whole interval $j \in [1, 67]$. This means that for states pp there are correlation relations with positive correlation coefficients. The distribution function of the Fermi-Dirac type $F_{55}(j)$ with increasing j (Fig. 1, a) varies randomly around the value of 0.1, goes to the stochastic peak at $j = 26$ with the value $F_{55}(26) = 0.3315$ and then again randomly changed by another law near the value of 0.1. The distribution function of the $F_{77}(j)$ with increasing j (Fig. 1,c) also varies randomly near the value of 0.1, comes to a peak at the other stochastic value of $j = 42$ with the same value of $F_{77}(42) = 0.3315$ and then again changes randomly by another law near the value of 0.1. In this case the values of the functions of $F_{55}(j)$, $F_{77}(j)$ in the peaks do not exceed the value of 0.5, which is typical for the ground state Fermi-system. The

distribution functions of Bose-Einstein type $f_{55}(j)$, $f_{77}(j)$ (Fig. 1,b,d) randomly change with increasing j near the population number equal to 10, in separate planes the peaks with large population numbers are observed. Such a behavior of functions $f_{55}(j)$, $f_{77}(j)$ indicates that the ground state of a Bose-system is populated (the population number greater than 1). The global minima with the values $f_{55}(26) = f_{77}(42) = 2.0162$ are observed in the points at which the main peaks of the functions $F_{55}(j)$, $F_{77}(j)$ are observed. The above values of the functions in global minima and main peaks indicate that the correlations in both ground and excited states of both Bose- and Fermi-systems are taken into account.





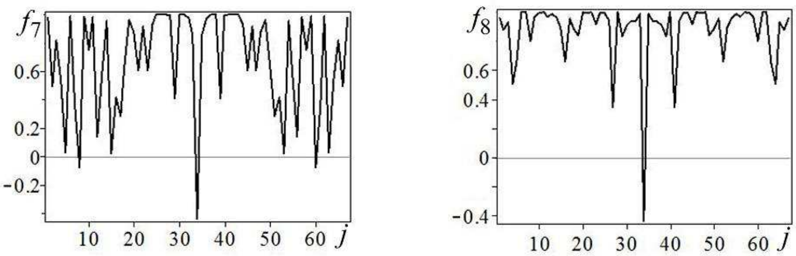
g h

Fig. 1. Dependencies of the distribution functions of the Fermi-Dirac type (a, c, e, g) and Bose-Einstein type (b, d, f, h) on j for mixed states *pp*

In this case, the autocorrelation function K_{55} describes a forward wave, and the autocorrelation function K_{77} describes a backward wave. The distribution functions of the Fermi-Dirac type $F_{66}(j), F_{88}(j)$ with increasing j (Fig. 1,e,g) vary randomly around 0.5. The values of the functions in individual peaks are higher than 0.5, which is typical for inverted states of Fermi-systems. The distribution functions of Bose-Einstein type $f_{66}(j)$, $f_{88}(j)$ (Fig. 1,f,h) randomly change with increasing j near the occupation numbers from 0 to 10, in separate planes the peaks with large population numbers are observed.

Accounting ordering pair operators in (1), (2) (the displacement and density of states of the lattice nodes) in the correlation function (6) - (9) leads to different distribution functions (10) - (13), as confirmed by numerical simulations (Fig. 1).

The dependencies of the distribution functions with mixed statistics (18) on an integer index j of a nodal plane for pure states at $r = 7,8$ are shown in Fig. 2.



a b

Fig. 2. Dependencies of the distribution functions with mixed statistics on j for pure states

At some points j changes sign at functions f_7, f_8, which confirms the presence of a mixed statistics. In this case functions f_r and f_r' may be interpreted as Fermi-Dirac type distribution functions for those areas of changes for j, where $K_r > 0$, and at $K_r < 0$ as Bose-Einstein type distribution functions in the main and excited states, respectively. Note the pronounced stochastic behavior of the amplitudes $|M_r|$ and phases μ_r have of averaged functions $M_r = Sp\hat{M}_r = =|M_r|\exp(i\mu_r)$.

The possibility of changing the sign of real parts of the first order complex correlation functions $K_{pq}(j), C_{pq}(j)$ (6), (7) and second order correlation functions $G_{pq}(j)$, $g_{pq}(j)$ (14), (16) is also confirmed by the results of the numerical simulations.

4. Conclusions

The numerical simulation has confirmed the theoretical conclusion of the presence of a mixed statistics: the change of the statistics from Fermi-Dirac type to the statistics of Boze-Einstein type for separate internal nodal planes of the bulk lattice. The analysis of the distribution functions of the occupation numbers for mixed states shows that particular nodal planes may be in inverse structural states.

Based on the analysis of the correlation functions of the first and second order a possibility of changing the sign of real parts of the correlation functions is shown. This indicates a possible change in the nature of the interaction (attraction or repulsion) between lattice nodes within a single nodal plane as well as between different planes.

Accounting ordering pair operators (displacement and density of states the lattice nodes) in the correlation function has the effect of deviations of the initial distribution function.

References

1. M.O Scully, M.S. Zubairy. *Quantum Optics*. Cambridge: Cambridge Univ. Press, 1997.
2. W. Paul. Electromagnetic traps for charged and neutral particles. *Rev. of Modern Physics* **62,** 3: 531-543, 1990.
3. M.H. Anderson, J.R. Ensher, M.R. Matthews et al. Observation of Bose-Einstein condensation in a dilute atomic vapor. *Science* **269,** 5221: 198-201, 1995.
4. S. Gleyzes, S. Kuhr, C. Guerlin et al. Quantum jumps of light recording the birth and death of a photon in a cavity. *Nature* **446**: 297-300, 2007.
5. C.W. Chou, D.B. Hume, T. Rosenband, D.J. Wineland. Optical clocks and relativity. *Science* **329**: 1630-1633, 2010.
6. J. Erhart, S. Sponar, G. Sulyok. Experimental demonstration of a universally valid error-disturbance uncertainty relation in spin measurements. *Nature Physics* **8**: 185-189, 2012.
7. A. Perrin, R. Bücker, S. Manz. Hanbury Brown and Twiss correlations across the Bose-Einstein condensation thereshold. *Nature Physics* **8**: 195-198, 2012.
8. K.K. Gomes, W. Mar, W. Ko, F. Guinea et al. Designer Dirac fermions and topological phases in molecular graphene. *Nature* **483,** 7389: 306-310, 2012.
9. 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.

10. 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.
11. 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.
12. 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.
13. V.S. Abramov. Inverse structural states of the stochastic deformation field of fractal dislocation. *Book of Abstracts 4th Chaotic Modeling and Simulation International Conference (CHAOS 2011), May 31 - June 3, 2011, Agios Nikolaos, Crete Greece*. p. 10, Greece, 2011.
14. H.-J. Stockmann. *Quantum Chaos. An Introduction.* Cambridge Univers. Press, 1999.
15. V.S. Abramov. Features of statistical properties of the deformation field of the fractal dislocation. *Bul. of Donetsk Nat. Univers*. Ser. **A,** 1: 105-113, 2012.
16. S.G. Samko, A. Kilbas, O. Marichev. *Fractional Integrals and Derivatives. Theory and Applications*. Gordon and Breach Sci. Publ., New York et alibi, 1990.
17. B.B. Mandelbrot. *The Fractal Geometry of Nature*. Freeman, New York, 1982.