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GENERALIZED HURST EXPONENT OF THE CARBON THIN FILM SURFACE

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Self-similar structure of the carbon thin film surface, obtained by magnetron sputtering, is investigated numerically. Statistical parameters are calculated within two dimensional multifractaldetrended fluctuation analysis. The numerical model of the surfaces under investigation was build from the SEM images of the carbon thin film. It is shown that the self-similarity in surface structure preserves through different resolutions of the SEM images.

Keywords: *SELF-SIMILARITY, CARBON THIN FILMS, HURST EXPONENT, FRACTAL DIMENSION.*

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1. INTRODUCTION

Self-similar or self-affine structures are widely presented in all areas of the nature science [1]. The self-similarity means that the each segment of the initial set has the same structure as the whole object. The properties of such systems can be described by special parameters, like fractal dimension (or set of dimensions in case of complex structures [2]), Hurst exponent and other [1, 2]. Most common examples of the geometric fractals are the Cantor and Serpinsky sets, the Koch curve and many others objects [2]. Self-similarity appears not only in topological structure of the objects, also the phase space of the complex stochastic systems often has a hierarchical structure with non participant regions [3].The stochastic fractals can be illustrated through the Lorenz attractor sand nonstationary time-series [4, 5].

Self-similar surfaces play the important role in surface contacts. Morphologies of these surfaces can appear to be quite different depending on the scale with which they can be observed. It can be shown that concepts like roughness are replaced by exponents that refer not to the roughness, but to the fashion in which the roughness changes when the observation scale itself changes [6]. The self-similarity of surfaces can be produced by the fracture or by the mechanical processing. Surface can be formed as a result of a deposition process, shrink due to erosion or etching, propagate through inhomogeneous media.Fractal dimension of such structures is usually determined by obtaining the photographs taken at various zoom levels, with subsequent application of the photograph at a square grid and numerical analysis.

In proposed article we present the investigation of the self-similar structure of the carbon film surface by numerical methods of scaling analysis. Our calculations are based on the algorithm mofmulti fractal

detrended fluctuation analysis (MF-DFA) [7], that differs from the standard box-counting based procedures of the fractal dimension estimation [8].The standard methodic gives precise results only for deterministic self-similar objects with explicit numerical model, and has a large error when applying to the surface models with discreet range of the coordinates [9]. The MF-DFA algorithm initially was developed for investigation of the time series as a one-dimensional self-similar set [4], and later generalized for more complicated objects analysis [7]. Applying MF-DFA algorithm to the self-similar surface model as to two-dimensional time series allows one to obtain a quantitative characteristic of the surface structure.

In the opening section of the paper we briefly describe the object of our research – carbon thin film, obtained through magnetron sputtering, and the possible way for numerical simulation of its surface structure. Next we refer the main steps of the MF-DFA algorithm and present the results of our calculations, comparing them for different parts of the surface sample. Our works ends with summation of the performed investigations.

2. THIN FILMS UNDER INVESTIGATION

Carbon condensates were obtained by deposition of the ion-sputtering substance onto (001) KCl facets according to original technique [10-14]. As a result the high porous carbon thin films were obtained. The SEM images of the condensates at different scale resolution are shown in Fig. 1.

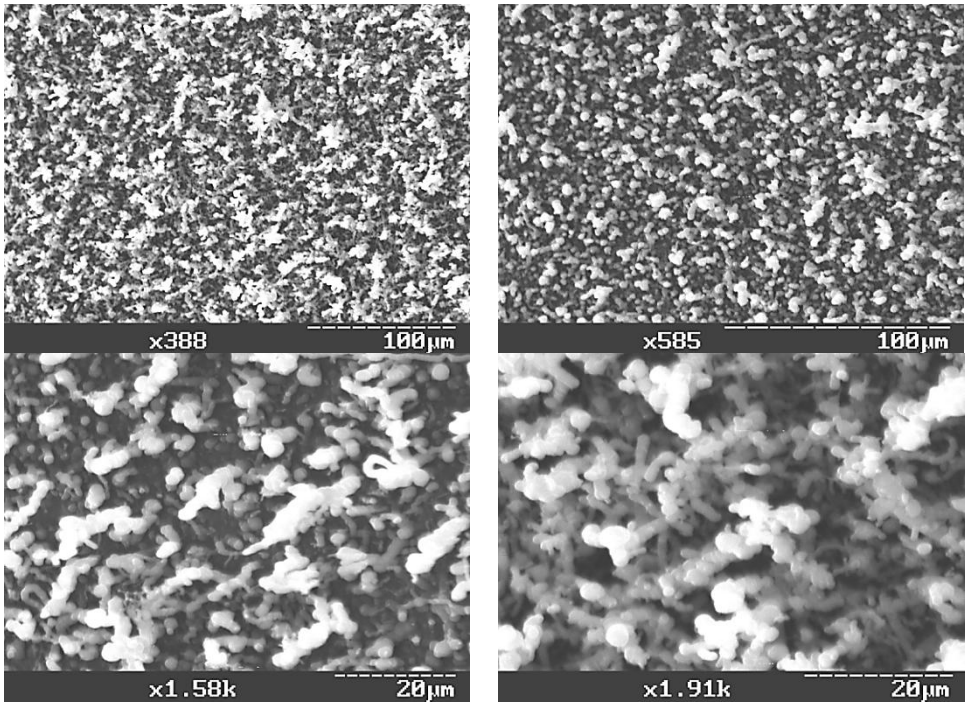

Fig. 1 *– SEM images of the carbon thin films at different scale resolutions* [14]

In order to investigate the self similarity in the structure of the surfaces we select the four SEM pictures of the surface at different microscopic

zoom, specified at the photos in Fig. 1. For each SEM image a numerical model was build. The image was presented by a surface in Cartesian coordinates, where each point defined by the numbers and brightness of the pixel in related image. Thus, the effective height of the surface model varies in the [0, 1] range, where zero height presents the absolutely dark (i.e. black) pixel. Example of the surface image and corresponded numerical model are presented in figure 2.Making use of the developed model allows for calculation of the generalized Hurst exponent within the two-dimensional MF-DFA algorithm [7].

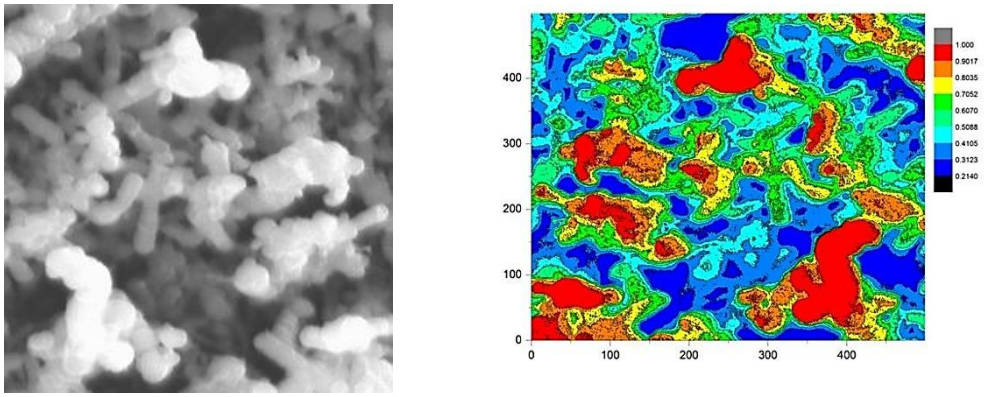

***Fig. 2** – Fragment of the SEM image of the carbon thin film (upper panel) and related numerical model (lower panel)*

3. IMAGE ANALYSYS METHODOLOGY

All surfaces were investigated within two dimensional multifractal detrended fluctuation analyses (MF-DFA) methodology [7]. This algorithm allows for calculation of the main parameter of the self similar structure, such as generalized Hurst exponent through the following numerical procedure [7].

Self-similar surface is considering as a two-dimensional data array X (i, j), where in dices i, j has a discrete values $i = 1,2,\ldots, M$ and $j = 1,2,\ldots, N$. This surface fragmented into $M_s \times N_s$ non overlapping segments of the size $s \times s$, where $M_s = [M/s]$ and $N_s = [N/s]$ are integer numbers.

Denoting each segment through υ, ω, the cumulative sum

$$u_{\upsilon\omega}(i,j) = \sum_{k_1=1}^{i} \sum_{k_2=1}^{j} X_{\upsilon\omega}(k_1,k_2), 1 \le i,j \le s, \qquad (1)$$

is calculated for all segments υ, ω.

Next step is a detrending procedure for the obtained surface $\tilde{u}_{\upsilon\omega}(i,j)$. The trend can be removed by the fitting procedure, when it determines by some smooth polynomial function $\tilde{u}_{\upsilon\omega}(i,j)$. There are many possible expression of the $\tilde{u}_{\upsilon\omega}(i,j)$ function [7], we chose the simplest one, in order to reduce the computational time:

$$\tilde{u}_{\upsilon\omega}(i,j) = ai + bj + c \tag{2}$$

where a, b, c – coefficients, defined by list-squares fitting algorithm. It should be mentioned, that more complicated forms of $\tilde{u}_{\upsilon\omega}(i,j)$ does not provides any significant increasing of the precision of the method, but noticeably increase computational time [7]. After detrending we arrive at residual function:

$$\varepsilon_{\upsilon\omega}(i,j) = u_{\upsilon\omega}(i,j) - \tilde{u}_{\upsilon\omega}(i,j)\,, \tag{3}$$

and a dispersion of the υ, ω segment of lengths:

$$F^2(\upsilon,\omega,s) = \frac{1}{s^2}\sum_{i=1}^{s}\sum_{j=1}^{s}\varepsilon^2_{\upsilon\omega}(i,j) \tag{4}$$

Dispersion of the all segments is calculated through averaging over all surfaces:

$$F_q(s) = \left\{\frac{1}{M_s N_s}\sum_{\upsilon=1}^{M_s}\sum_{\omega=1}^{N_s}[F(\upsilon,\omega,s)]^q\right\}^{1/q}, \tag{5}$$

where q is a deformation parameter, initialized to increase the role of the segments with small (when $q < 0$) or high ($q > 0$) fluctuations $F^2(\upsilon, \omega, s)$ respectively [4]. A $t_q = 0$ expression (5) takes form [6]:

$$F_0(s) = \exp\left\{\frac{1}{M_s N_s}\sum_{\upsilon=1}^{M_s}\sum_{\omega=1}^{N_s}\ln[F(\upsilon,\omega,s)]\right\}, \tag{6}$$

according to l'Hôpital's rule. For statistically correct result s values must be varied in the range from $s_{min} \approx 6tos_{max} \approx \min(M, N) / 4$.The dispersion (5) and the segment size s connected through a scaling relation:

$$F_q(s) \sim s^{h(q)}\,, \tag{7}$$

where, $h(q)$ is a generalized Hurst exponent. If the object under investigation has a self similar structure, the dependence (7) must be linear in logarithmic scales. Examples of relation (7) for the surfaces of the carbon thin films are presented in Fig. 3.

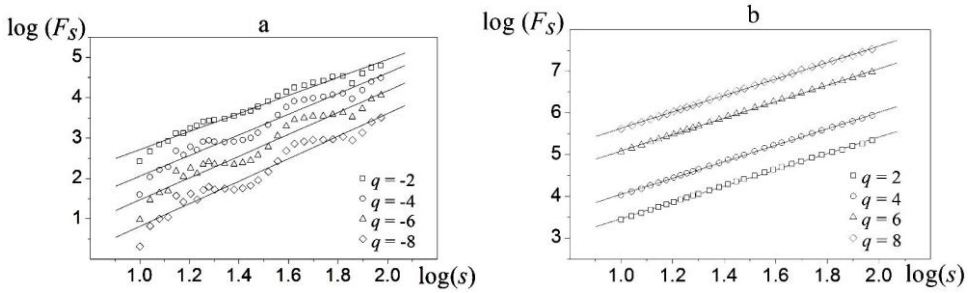

Fig. 3 *– Relation (7) in logarithmic scales for the surface of the carbon thin films plotted at different negative (a) and positive (b) values of the deformation parameter q*

As it follows from the figure, dependence (7) has a clear linear form only for $q > 0$ values, while in opposite range the calculations are expected to give a large error.

4. RESULTS AND DISCUSSION

The generalized Hurst exponent was calculated for all surfaces, shown in Fig. 1. According to the structure of the fractal objects, the Hurst exponent of the self-similar surface are expected to be independent from the resolution scale. The results of the calculations are shown in Fig. 3.

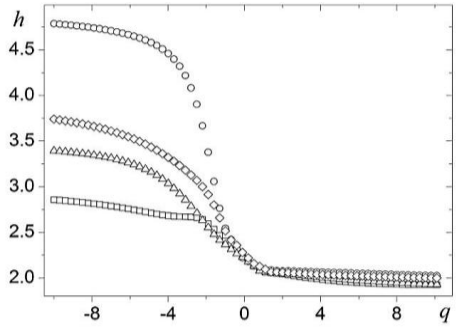

Fig. 4 *– Hurst exponent of the carbon thin film surface at different SEM images resolutions (different symbols relate to the different microscopic scale zoom: squares* – 585*, circles* – 1910*, triangles* – 383 *and diamonds* – 1580*)*

As it can be seen from the figure, the calculated parameters for different resolution scale of the surfaces are almost coinciding in $q \geq 0$ region, and differs from each other for $q <$ values, i.e. self-similarity in surface structure exist while $q \geq 0$, and breaks at $q < 0$. This result can be explained by the statistical meaning of the fluctuation function (5), when $q < 0$, the main contribution in (5) is made by the segments v, ω with small fluctuation (4) (namely $F^2(v, \omega, s) << 1$), due to the power q.

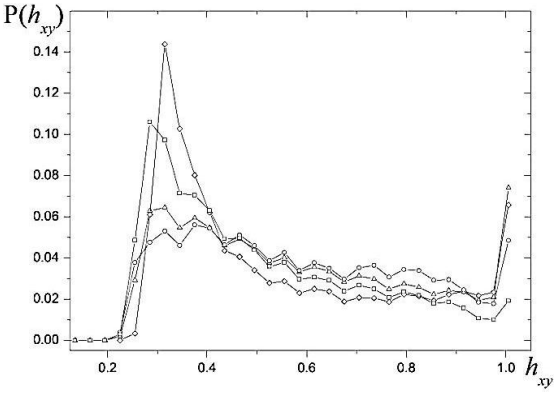

Fig. 5 *– Density distribution of the effective heights of the surfaces at different SEM images resolutions (different symbols relate to the different microscopic scale zoom: squares* – 585*, circles* – 1910*, triangles* – 383 *and diamonds* – 1580*)*

Such $F^2(\upsilon, \omega, s)$ values are calculated in segments where the surface height coordinates are maximally close to the smooth function $\tilde{u}_{\upsilon\omega}(i,j)$ (in general, $F^2(\upsilon, \omega, s)$ depends on the segments size s, but since the whole set $s_{\min} \le s \le s_{\max}$ is considered for every q value, this dependence is insignificant). Noticeably, since the fluctuation $F^2(\upsilon, \omega, s)$ is not equal to zero for any segment υ, ω [7], totally smooth areas of the surface with any size $s \times s$ are never appears. The segments with $F^2(\upsilon, \omega, s) << 1$ can be related to those areas of the SEM images, that appears to be enormously dark or bright or corrupted because of image noises and defects of the scanning microscopy imaging. There is no strong self-similarity in the structure of these areas in the surface, and this situation causes the difference between Hurst exponents in the $q < 0$ region. To verify this assumption we calculate the distribution of the effective height h_{xy} over numerical models of each surface (figure 5). As it can be seen from the shown dependencies, most significant differences between distributions are observed for most dark and bright areas of the SEM images (minimum and maximum heights of the surface respectively). This feature can be the reason of the difference between Hurst exponents at $q < 0$.

5. CONCLUSIONS

Above consideration shows, that the surface of the carbon condensates has the self-similar structure. This conclusion follows from the approximately the same Hurst exponent for different scale of the surface observation at positive deformation parameter q. Nevertheless, when $q < 0$, calculated parameters are strongly distinguishing. We explain this situation by the statistical meaning of the fluctuation function (5) and q parameter, which negative values related to the small fluctuations of the surface roughness, i.e. the self – similarity parameters at $q < 0$ represent the small details of the SEM images and can include the technical noise, which are always present in the scanning microscopy. Hurst exponent is often used as a parameter of the surface roughness [15], thus, obtained dependencies also can be useful in studying of the physical properties of the thin films.

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