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STATISTICAL AND FRACTAL ANALYSIS OF RANDOM HEIGHT FUNCTION

Nanostructured semiconductor surfaces are commonly used for suppression of the light reflection. We prepared several kinds of surface structures on silicon substrate and analyzed the properties of the random height function used for the description of observed surface morphology. Statistical and fractal methods used in this analysis provide useful information for the optimization of the surface forming procedure. Multifractal analysis provides additional information about the surface morphology, not contained in the results of standard statistical methods. Numerical procedures used in the multifractal analysis were tested by using theoretical random height function created from large sets of Cantor numbers.

Keywords: *Multifractal analysis, statistical methods, semiconductor structures.*

1. Introduction

The properties of microstructure play an important role in fabrication of electronic and photonic devices, especially in solar cells [1]. In order to decrease the reflection losses and increase the absorption probability by light trapping in the solar cell structure random pyramidal textures are usually prepared at the semiconductor surface [2 - 8]. Pyramidal texture is formed by etching of the silicon surface and contains a large variety of surface shapes depending on the technological treatment. For characterization of the pyramidal surface morphology, the random height function $h(x,y)$ describing the height of atom above the reference plane at position (x,y) can be used. The characteristics of the random height function are visually apparent but not sufficiently described by conventional measures like mean value or standard deviation. The values of the random height function $h(x,y)$ can be experimentally obtained by the electron microscopy or by the scanning probe methods with atomic resolution [9, 10]. Experimental values of $h(x,y)$ posses a scale invariant structure. The particular kind of scale invariant structure in the experimental data $s(x)$ is defined by the power exponent H in an equation for scaling of observed data $s(cx) = c^H s(x)$. The complex shape of the random height function can be described by the fractal methods in this case [11 - 14]. The variations in scale invariant structure can be often observed in the experimental surface images. This indicates a multifractal structure of scanned surface image that is defined by a multifractal spectrum of power law exponents rather than a single power law exponent for monofractal.

In this paper we describe results of statistical and multifractal analysis of theoretical surface generated by using Cantor numbers [15] as well as the random height function of real semiconductor structures, observed with atomic resolution.

2. Multifractal analysis

For the description of the random height function properties the multifractal singularity spectrum $f(\alpha)$ and generalized fractal dimension D_q can be used. The box-counting method is often used for the multifractal analysis studied structure. The observed surface is divided into square areas with the size of side ε. In a selected area the probability measure is defined by

$$P_i(\varepsilon) \sim \varepsilon^{\alpha_i} \tag{1}$$

where a_i is singularity exponent. If $N(\alpha)$ is the number of surface areas in which P_i has singularity α_i in an interval $\alpha_i \in (\alpha, \alpha + d\alpha)$, then multifractal singularity spectrum $f(\alpha)$ is defined by equation

$$N(\alpha) \sim \varepsilon^{-f(\alpha)} \tag{2}$$

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Function $f(\alpha)$ can be interpreted as the fractal dimension of surface areas with singularity α. This definition is connected with the multifractal measure described by the multifractal singularity spectrum.

For the characterization of multifractal properties of the studied surface generalized fractal dimension D_q can be alternatively used. The *q-th* moment of the P_i measure is defined by the equation

$$D_q = \frac{1}{q-1} \lim_{q \to 0} \frac{\log \sum_i P_i(\varepsilon)^q}{\log \varepsilon} \tag{3}$$

In case when D_q does not depend on q then the studied surface $h(x,y)$ is monofractal. By using the Legendre transformation we obtain relation of $f(\alpha)$ and D_q in form

$$f(\alpha) = \alpha q - (q-1) D_q \tag{4}$$

For $q = 0$ we obtain Hausdorff fractal dimension

$$D_0 = -\lim_{q \to 0} \frac{\log N}{\log \varepsilon} = \lim_{q \to 0} \frac{\log N}{\log 1/\varepsilon} \tag{5}$$

By using L'Hospital's rule we obtain for $q = 1$

$$\begin{aligned} D_1 &= \lim_{q \to 1} \frac{1}{q-1} \lim_{\varepsilon \to 0} \frac{\log \sum_i P_i^q}{\log \varepsilon} = \\ &= \lim_{\varepsilon \to 0} \lim_{q \to 1} \frac{\sum_i P_i^q \log P_i}{\log \varepsilon \sum_i P_i^q} = \lim_{\varepsilon \to 0} \frac{\sum_i P_i \log P_i}{\log \varepsilon} \end{aligned} \tag{6}$$

Dimension D_1 corresponds to the entropy or information dimension. Lower value of D_1 indicate higher disorder of observed random height function $h(x,y)$.

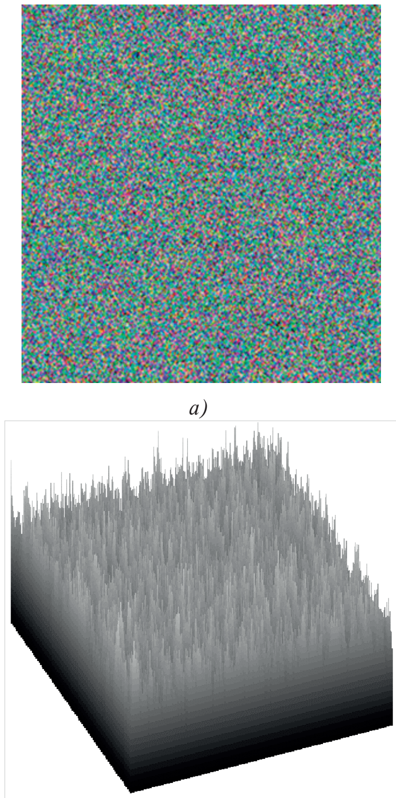
For $q = 2$ we obtain correlation dimension

$$D_2 = \lim_{\varepsilon \to 0} \frac{\log P_i(\varepsilon)^2}{\log \varepsilon} \tag{7}$$

suitable for an identification of the surface homogeneity. The higher degree of the surface homogeneity, the higher value of D_2 is observed [12, 13, 16, 17].

3. Results and discussion

For analysis of multifractal properties of the $h(x,y)$ function, we generated theoretical surface by using Cantor numbers. We determined values of the $h(x,y)$ function by random selections from large Cantor sets $C(n)$. Cantor sets were constructed by dividing of unit interval into three subintervals ($C(3)$), five ($C(5)$), seven ($C(7)$) and nine subintervals ($C(9)$). By the random selection (with uniform distribution) from these Cantor sets the different $h(x,y)$ functions representing surface areas of various size were constructed. Random surface generated by this way is shown in Fig. 1.



a)

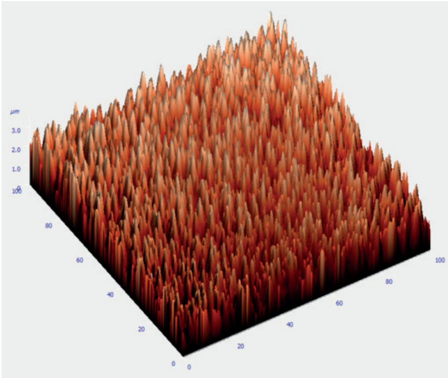
b)

Fig. 1 Random height function generated from Cantor set numbers $C(3)$; a) 2D plot, b) 3D plot

For computation of the P_i in (Equation 1) we used the box-counting method

$$P_{ij} = \frac{h_{ij}}{\sum h_{ij}} \tag{8}$$

where h_{ij} is the mean value of the $h(i,j)$ function in the box $box(i,j)$. By using this probability we computed generalized fractal dimension D_q (Equation 3) and multifractal spectrum $f(\alpha)$ (Equation 4). The results of developed numerical procedures show expected behaviour for multifractal structures of theoretical Cantor test surfaces and were used for analysis of real semiconductor surfaces. In Fig. 2 two distributions of pyramidal textures formed on flat silicon surface are shown. In pyramidal structure d1 a quasi homogeneous distribution of pyramidal shapes was formed whereas in structure d2 dominant fraction of small pyramids with random occurrence of very high pyramids was created.



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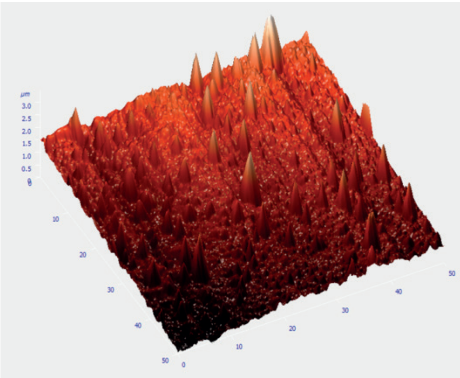

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Fig. 2 Pyramidal structures prepared on Si surface: a) distribution d1, b) distribution d2

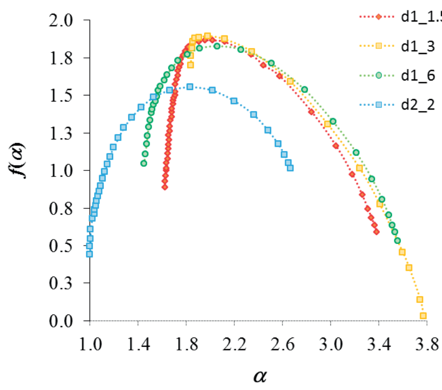
Statistical characteristics of the random height function $h(i,j)$ values obtained by the atomic force microscopy experiment for these pyramidal structures are shown in Table 1.

Statistical characteristics of the experimental random height function Table 1

Distribution		d1	d2
Max	nm	2946.51	2206.76
Peek-to-peek S_y	nm	2946.51	2206.76
10-point height S_z	nm	1483.12	1069.98
Average roughness S_α	nm	1417.75	664.146
Mean square roughness S_q	nm	461.827	146.431
Coefficient of variation S_q/S_α		0.326	0.22
Skewness S_{sk}		0.154	2.467
Kurtosis S_{ku}		-0.389	11.761

The values of these statistical characteristics can be used in study of the surface roughness properties. Coefficient of variation is a relative measure of variability between structures with different averages. For distribution d1 this indicates higher surface roughness. Higher value of the skewness for distribution d2 is influenced by higher inhomogeneity of the pyramidal shapes in this distribution (dominant fraction of small pyramids). Negative value of kurtosis for distribution d1 shows low influence of different pyramidal shapes onto the statistical properties of d1 distribution and high value of kurtosis for distribution d2 indicates the presence of abnormally high pyramidal shapes at observed surface.

Statistical analysis provides useful information about the random height function properties. Supplementary information can be obtained by using multifractal methods. In Fig. 3 results of multifractal analysis of four pyramidally textured surfaces are shown.



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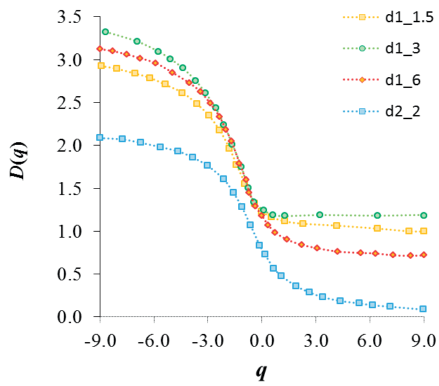

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Fig. 3 Results of multifractal analysis of pyramidal texture with maximal heights of pyramids 1.5, 1.3, 1.6, and 2.2 µm: a) multifractal singularity spectrum $f(\alpha)$, b) generalized fractal dimension $D(q)$

We analyzed distributions d1 and d2 where maximal height of the pyramid equals 3 µm and we studied also distribution d1 with maximal height of pyramidal shapes 6 µm and 1.5 µm. Generalized fractal dimension D_q curves show decreasing trend significant for multifractal surface morphology. In plot of the D_q curves we observe important difference between characteristics for d1 and d2 distribution. Surface structure d2 has significantly lower D_q values in comparison to homogeneous distribution d1 for all q values. Value of dimension D_0 connected with traditional fractal dimension is very similar for all pyramidal distributions (with different heights of pyramids). On the other side significant differences can be seen in comparison of distributions d1 and d2. Lower value of dimension D_1 for distribution d2 indicates higher disorder in this pyramidal distribution (higher randomness) in comparison to d1 distribution. Maximal value of the correlation dimension D_2 indicates the highest homogeneity of the observed surface.

Multifractal characteristics are therefore very sensitive to small changes in the surface height function and in the distribution of pyramidal shapes. Different shapes of the D_q curves enable us to distinguish reliably between the properties of different distributions d1 and d2 as well as between small changes in the same distribution of pyramidal shapes (for example, for distributions type d1 with different heights of pyramids). The obtained results can be therefore used for the optimization of technological steps of surface texture forming procedure.

Multifractal singularity spectrum $f(\alpha)$ has concave shape typical for multifractal morphology. The maximal height of the $f(\alpha)$ spectrum is given by the D_0 value and the width of $f(\alpha)$ spectrum corresponds to the variability of shapes of the morphological objects. Symmetry of the $f(\alpha)$ curve is different for distribution d2, which indicates higher non-uniformity of distribution d2 in comparison to distribution d1.

In Fig. 4 multifractal spectrum $f(\alpha)$ curves for thin nanocrystalline layers formed by etching of silicon surface in the HF acid in contact with the Pt electrode are shown.

The analyzed structures were etched for 10, 20, and 30 seconds and values of the random height function were obtained by the scanning electron microscope with magnification 2000. From the shape of $f(\alpha)$ curves we can see, that the surface morphology develops primarily in the first stages of etching procedure (during the first 20 seconds). With the prolongation of etching time the development of surface morphology stabilizes.

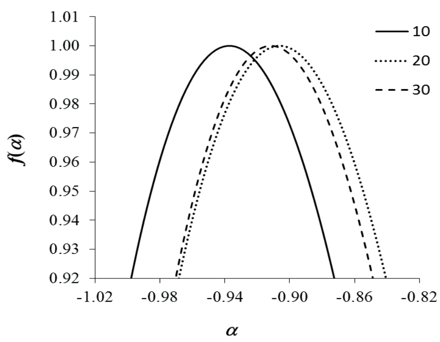

Fig. 4 Multifractal spectrum f(α) curves of the nanocrystalline Si layers

4. Conclusions

Statistical and multifractal analysis provides information about the shape of morphological objects development as well as about the intensity of modification of treated surface morphology. Multifractal analysis is a suitable tool for study of the random height function properties, providing additional information about the surface morphology, not contained in the results of standard statistical methods.

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