OFSTATISTICAL AND FRACTAL PROPERTIES OF SEMICONDUCTOR SURFACE ROUGHNESS

S. Jurečka[1], M. Jurečková[2], H. Kobayashi[3], M. Takahashi[3], M. Madani[3] E. Pinčík[4]

[1]*DEF FEE, Žilina University, Nálepku 1390, 03101 L. Mikuláš,Slovakia, e- mail: jurecka@lm.uniza.sk*
[2]*Academy of Armed Forces of Gen. M. R. Štefánik, Demänová 393, 03101 L. Mikuláš, Slovakia*
[3]*DFCM ISIR, Osaka University, Mihogaoka 8-1, Ibaraki, Osaka 567-0047, Japan*
[4]*Institute of Physics SAS, Dúbravská cesta 9, 84511 Bratislava, Slovakia*

Summary Surface morphology evolution is of primary significance for the thin-film growth and modification of surface and interface states. Surface and interface states substantially influence the electrical and optical properties of the semiconductor structure. Statistical and fractal properties of semiconductor rough surfaces were determined by analysis of the AFM images. In this paper statistical characteristics of the AFM height function distribution, fractal dimension, lacunarity and granulometric density values are used for the surface morphology of the SiC samples description. The results can be used for solution of the microstructural and optical properties of given semiconductor structure.

1. INTRODUCTION

One of the consequences of the semiconductor surface and thin film structures preparation is the evolution of roughness. Statistically rough semiconductor surfaces generated in non-equilibrium growth processes have attracted much interest because understanding of the growing surface morphology evolution is of primary significance for the thin-film growth and modification of surface and interface states. Surface and interface states substantially influence the electrical and optical properties of the semiconductor structure [1-4].

Atomic force microscopy (AFM) is well suited for the measurement of surface roughness in the nanometer scale. In this paper, an AFM was employed to directly measure the surface roughness of the SiC samples with various types of irregularities at the surfaces. Statistical characteristics of the surface roughness and fractal properties of the sample surfaces are reported and discussed in connection with the determination of the optical parameters of the studied structure.

In the visible and infrared region the optical properties of solids are determined mainly by the states of the valence electrons. Important role play also vibrational and rotational movements of molecules. In this region optical processes in semiconductors take place mainly between the conduction and valence bands. Optical reflection and absorption spectroscopy is therefore a convenient way of studying the band structure. Surface roughness changes the spectral reflectance function of the boundary between two media. In our approach the optical parameters computations are based on the modification of the Fresnel spectral reflection coefficient by the surface roughness characteristics [5]. In this work the properties of the surface roughness are determined by the statistical and fractal methods.

2. THEORY

Because of the complexity the rough surface is often viewed as a realization of a random process. In the application of this approach the displacements of the surface points from the reference plane are modeled as a random surface and characterized by appropriate distribution of the height function (roughness) values z [6-7]. The normal distribution is often used as a model for the surface roughness description. The density function of the normal distribution depends on two parameters, mean μ and standard deviation σ

$$f(z)=\frac{1}{\sigma\sqrt{2\pi}}\exp\left[-(z-\mu)^2/2\sigma^2\right] \qquad (1)$$

Departures from normality often take the form of asymmetry. For a normal distribution the third central moment equals zero:

$$\int_{-\infty}^{\infty}(z-\mu)^3 f(z)\,dz=0\,. \qquad (2)$$

Asymmetry of the roughness distribution can therefore be tested by using the sample coefficient of skewness:

$$R_{sk}=\frac{\sum_{i=1}^{n}(z_i-\overline{z})^3}{n\,s^3}\,, \qquad (3)$$

where n is the number of height function values, s is the sample standard deviation and $\overline{z}$ is the sample mean. Large values of $|R_{sk}|$ implicate deformation of the roughness distribution shape. Symmetric distributions can depart from normality by being heavily- or light-tailed or too peaked or flat in the center. These deformations can be detected by the sample coefficient of kurtosis [8]:

$$R_{ku}=\frac{\sum_{i=1}^{n}(z_i-\overline{z})^4}{n\,s^4}\,. \qquad (4)$$

Real surfaces possess a wide range of roughness scales. The existence of various scales could alter the dimension of the surface and therefore can lead to errors in the estimation of the statistical characteristics of the surface.

The basic concept for description of the rough surface with symmetric scaling is fractal dimension D_F [9-10]. Fractal is a geometric shape that can be divided into subparts, each of which is a copy of whole. This property of fractals is called self-similarity. This means that self-similarity of the chosen element at a variable magnification scale can be observed. A magnified view of one part of the rough surface do not precisely reproduce its whole structure but has the same qualitative appearance. A complex character of the semiconductor rough surface is often described by more than one fractal dimension. Because the rough surface does not exhibit a form of purely self-similar fractal, the self-similarity is local only. The surface irregularity distribution changes depending on the studied region. Concentration of large surface irregularities often occurs in a few regions and concentration of small irregularities in many regions. Therefore the most suitable method for the surface properties description is a multifractal analysis. In this work we use the method of computing the $f(\alpha)$ multifractal spectrum developed by Chhabra and Jensen [11]. The $f(\alpha)$ spectrum is the dimension of the theoretical support of a particular measure. In this method the probability of finding an ith fragment of the analyzed surface region is expressed by the formula $P_i(\delta)=A_i(\delta)/A_T(\delta)$, where $A_i(\delta)$ is the area in an ith box with δ scale and $A_T(\delta)$ is the total area measured in δ scale. Fractal dimension is computed by formula

$$D_F=\frac{1}{q-1}\lim_{q\to 0}\frac{\log\sum_{i=1}^{N}\left[P_i(\delta)\right]^q}{\log\delta} \tag{5}$$

where $q\in(-\infty,\infty)$, N is total number of boxes necessary for covering A_T. In terms of probability P_i a one-parameter family of normalized measure ζ is constructed

$$\zeta(q,\delta)=\frac{P_i(\delta)^q}{\sum_{i=1}^{N}P_i(\delta)^q}\,. \tag{6}$$

The fractal dimension of the subset $f(q)$ is determined by equation

$$f(q)=\lim_{\delta\to 0}\frac{\sum_{i=1}^{N}\zeta_i(q,\delta)\log\zeta_i(q,\delta)}{\log\delta} \tag{7}$$

indexed with the exponent $\alpha(q)$

$$\alpha(q)=\lim_{\delta\to 0}\frac{\sum_{i=1}^{N}\zeta_i(q,\delta)\log P_i(q,\delta)}{\log\delta} \tag{8}$$

The multifractal analysis describes the statistical properties of the measure in terms of its distribution of the singularity spectrum $f(\alpha)$ corresponding to its singularity strength α. If the shape of $f(\alpha)$ curve is humped, than the scaling of the surface is considered multifractal. If the spectrum $f(\alpha)$ converges, the surface is considered mono- or non-fractal. Curve $f(\alpha)$ is convex with a single inflexion point at the maximum with $q = 0$.

Another measure of the rough surface inhomogeneity in an AFM scan of the surface is lacunarity Λ [12]. Lacunarity is strongly related to the size distribution of the gaps on the fractal. It quantifies deviation from translational and rotational invariance by describing the distribution of gaps within a set at multiple scales. Fractal dimension and lacunarity work together to characterize the rough surface properties. Surfaces with identical fractal dimension can be distinguished by their lacunarity and vice versa. In this work lacunarity is computed by regular box counting technique [13].

Structure objects observed at the semiconductor surface by the AFM technique can be characterized by the particle size distribution. This distribution can be extracted from the AFM image by counting number of pixels corresponding to the morphological structuring elements at the surface. Granulometric density function is often referred as pattern spectrum of the image. Granulometric density G is in this work computed by using particle segmentation based on binary thresholding technique [14].

3. EXPERIMENTAL RESULTS

Statistical and fractal properties of rough semiconductor surfaces were analyzed on the series of SiC samples with surfaces treated by several technological operations. After cleaning the SiC wafers using the RCA method and etching with dilute hydrofluoric acid, the SiC wafers were annealed using an electrical furnace, in a pure hydrogen (grade 99.999% purity) atmosphere at 400 °C for 20 min. using a quartz glass tube as containment. Low temperature hydrogen annealing can improve the SiC MOS devices properties [15]. Surface roughness function values were measured by nanoscale hybrid AFM microscope Keyence VN-8010 in a tapping mode. Surface image is in this mode produced by analyzing the interaction of the oscillating AFM cantilever with the sample surface. Scanned area was set to 100 x 100 μm^2 (series a), 50 x 50 μm^2 (series b) and 10 x 10 μm^2 (series c). The surface irregularities of analyzed samples were of lamellar shape (sample A after the H_2 treatment, Fig. 1) and peak shape (sample B before the H_2 treatment, Fig. 1).

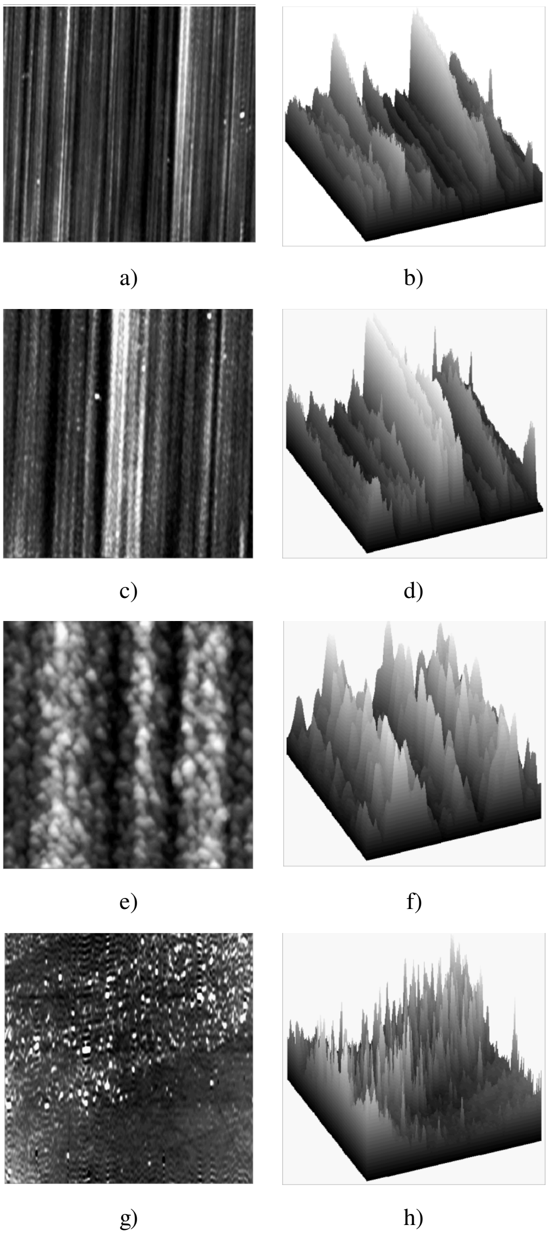


Fig. 1: Rough surfaces of SiC samples measured by Keyence AFM microscope: a) sample A, area 100 x 100 μm^2, b) 3D surface plot of this area, c) sample A 50 x 50 μm^2, d) 3D surface plot of this area, e) sample A, area 10 x 10 μm^2, f) 3D surface plot of this area g) sample B, area 100 x 100 μm^2, h) 3D surface plot of this area.

For all sample surfaces the following statistical characteristics were determined: rms roughness R_{rms}, average roughness R_a, coefficient of skewness R_{sk} (eq. 3), coefficient of kurtosis R_{ku} (eq. 4). Statistical analysis results are summarized in Table 1. Fractal properties of the surface structures were analyzed by computing the fractal dimension D_F and lacunarity Λ. Results of the fractal analysis - mean fractal dimension D_F and lacunarity Λ - are summarized in Table 2, Fig. 2 and Fig. 3.

Granularity density function G values determined for the sample series A and B are in Fig. 4.

Table 1: Statistical analysis results

sample	R_{rms}	R_a	R_{sk}	R_{ku}
A a	36.2993	25.3496	1.6585	4.3507
A b	48.8755	35.4961	1.4286	1.9424
A c	50.9687	42.2538	0.6811	-0.2706
B a	42.1513	28.8376	1.9797	4.7179
B b	40.4271	31.3483	0.9345	1.429
B c	49.1915	39.7254	0.3403	-0.0531

Table 2: Fractal analysis results

sample	mean D_F	Λ
A a	1.6269	431
A b	1.7841	605
A c	1.9016	654
B a	1.5111	205
B b	1.7024	828
B c	1.8814	2199

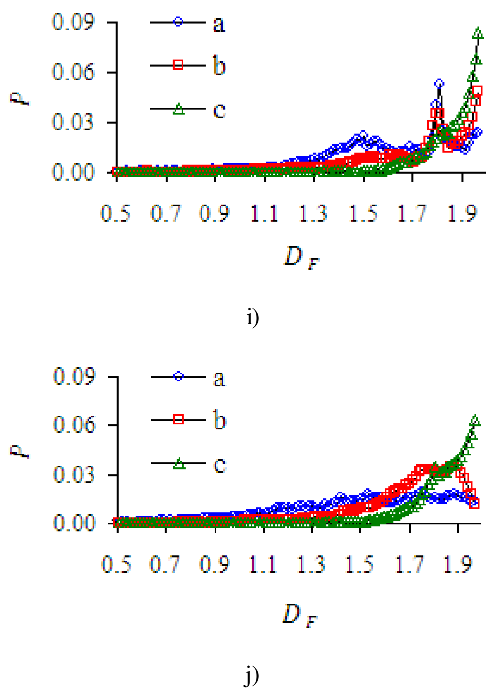
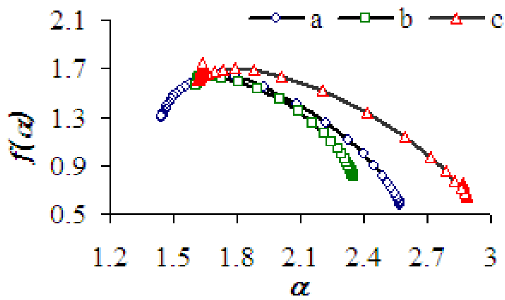
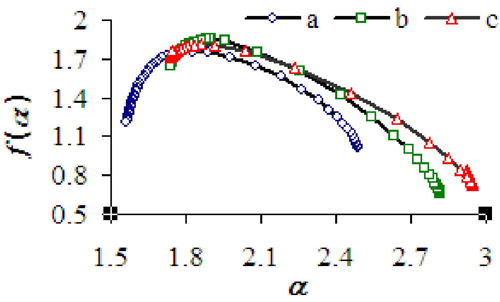


Fig. 2: Probabilities P of the surface fractal dimension D_F: i) sample series A, j) sample series B, a) area 100 x 100 μm^2, b) area 50 x 50 μm^2, c) area 10 x 10 μm^2.

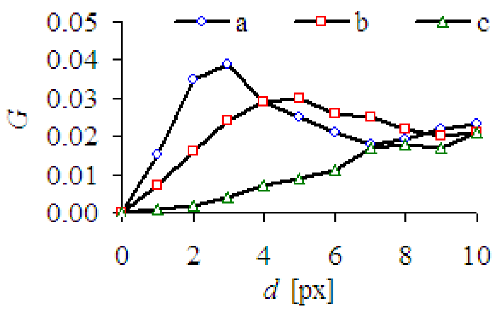


i)

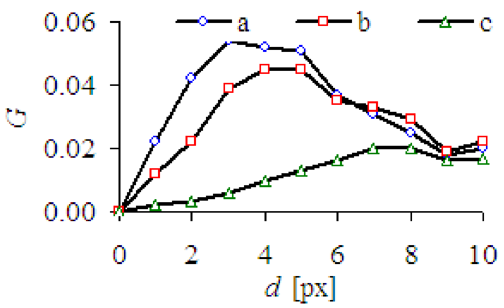


j)

Fig. 3: Multifractal spectrum: i) sample series A, j) sample series B, a) area 100 x 100 μm², b) area 50 x 50 μm², c) area 10 x 10 μm².



i)



j)

Fig. 4: Granularity density function G values: i) sample series A, j) sample series B, a) area 100 x 100 μm², b) area 50 x 50 μm², c) area 10 x 10 μm².

4. CONCLUSION

We used new statistical and fractal methods for the analysis of the SiC samples surface morphology. Surface roughness statistical characteristics strongly depend on the AFM microscope resolution. Average and rms roughness increase, skewness and kurtosis decrease with increasing of the resolution. It is therefore important to use identical AFM resolution for the comparative study of the sample series and adjust the resolution when studying individual surface objects. Skewness and kurtosis values differ from values of these coefficients for normal surface roughness distribution, where $R_{sk} = 0$ and $R_{ku} = 3$. Obtained skewness and kurtosis values indicate, that used sample treatment operations modified both the lamellar and peek shape structured surfaces in a systematic way. Positive skewness coefficient values signify that height function values smaller than mean value dominate in comparison to the normal distribution. High kurtosis coefficient values signify narrower height function distribution around the mean value in comparison to the normal distribution.

Fractal dimension changes with the AFM resolution moderately. Multifractal spectrum reveals multifractality at sample series A and B only for sample surfaces a) (the shape of $f(\alpha)$ curve is humped). The $f(\alpha)$ curve of the multifractal spectrum converges for surfaces b) and c) and therefore we can conclude that the surface looses its complexity with increasing the AFM microscope resolution. For implementation of the statistical and fractal analysis results into the following microstructural and optical methods the AFM resolution have to be carefully adjusted to ensure high complexity of the analyzed surface.

In the fractal dimension probabilities graphs the peak of D_F probability can be observed for lamellar structured surfaces. This peak can be interpreted as fractal evidence of the preferred structure pattern existence at given surface (lamellar chains).

Granulometric analysis shows degradation of the particle size distribution shape with increasing of the AFM resolution. At the atomic resolution individual structure patterns can be observed and the peak at particle size distribution curve disappears.

Statistical and fractal analysis provide information about the semiconductor surface structure objects. The AFM microscope resolution have to be chosen in accordance to the required complexity of the analyzed surface, that can be determined by the multifractal method. Information about the structure patterns properties can subsequently be used for the construction of microstructural and optical dispersion models as well as for the solution of other problems concerning the quality of the semiconductor surface.

Acknowledgement

This work was supported in part by the Slovak grant agency under grant VEGA 2/7120/27, JSPS Japan grant agency and AGA-01-2008 of MoD Slovak grant agency.

REFERENCES

[1] Kobayashi H., Takahashi M., Maida O., Asano A., Kubota T., Ivančo J., Nakajima A., Akimoto K.: Applied Surface Science 235, 2004, pp. 279-292.

[2] Yamahita Y., Asano A., Nishioka Y., Kobayashi H.: Phys. Rew. B. Vol. 59, No. 24, 1999, p. 15872-15881.

[3] Maida O., Asano A., Takahashi M., Iwasa H., Kobayashi H.: Surface Science 542, 2003, pp. 244-252.

[4] Asuha, Kobayashi T., Takahashi M., Iwasa H.., Kobayashi H.: Surface Science 547, 2003, pp. 275-283.

[5] Jurečka S., Pinčík E., Brunner R.: Applied Surface Science, Vol. 254, No. 12, 2008, pp. 3672-3676.

[6] Bass F.G., Fuks I.M.: *Wave scattering from statistically rough surfaces*. Pergamon Press., New York, 1979.

[7] Rice J.A.: *Mathematical Statistics and Data Analysis*. Thomson Books/Cole, Belmont, USA, 2007.

[8] Chinga, G., Johnssen, P.O., Dougherty, R, Lunden-Berli, E. and Walter, J.: J. Microscopy, Vol. 227, No. 3, 2007, pp. 254-265.

[9] Mandelbrot B.B.: *The fractal of nature*. Freeman, New York, 1982.

[10] Gouyet J-F.: *Physics and fractal structures*. Springer-Verlag, New York, 1996.

[11] Chhabra A., Jensen R.V.: Phys. Rev. Lett. 62, 1989, pp. 1327-1330.

[12] Plotnick R.E., Gardner R.H., Hargrove W.W., Prestegaard K., Perlmutter M.: Phys. Rev. E. Vol. 53, No. 5, 1996, p.5461-8.

[13] Allain C., Cloitre M.: Phys. Rev. A, 44, 1991, pp. 3552-3558.

[14] http://www.macbiophotonics.ca/imagej/particle_analysis.htm

[15] Im S-S., Terakawa S., Iwasa H., Kobayashi H.: *Nitric acid oxidation to form SiO2/3C-SiC structure at 120 °C*. Applied Surface Science, Vol. 254, No. 12, 2008, pp. 3667-3671.