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Simulation and Analysis of Surface Roughness of Soft Polymeric Materials by Fractals

Loreta MAČĖNAITĖ[1*], Vidmantas PEKARSKAS[1], Audrius ŽUNDA[2]

[1]*Faculty of Fundamental Sciences, Kaunas University of Technology, Studentų 50, LT-51368 Kaunas, Lithuania*
[2]*Faculty of Engineering, Lithuanian University of Agriculture, Studentų 15, LT-53362, Kaunas-Akademija, Lithuania*

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The surface roughness is important design factor for the adhesive bonds. Thus, in this work we have investigated the profiles of roughened surface of soft polymeric material. Five different grades of abrasive paper were used to produce different degrees of roughness on the monolithic butadiene-styrene rubber surface. The fractal model of surface roughness was proposed. It was determined that fractal dimension of profiles of roughened surface depends on grade of abrasive paper. It was shown that fractal dimension can be used to characterize the roughness of rubber surface.
Keywords: abrasion, surface roughness, correlation function, fractal dimension.

1. INTRODUCTION

Surface roughness plays an important role in many areas of science and technology. The degree of roughness is important design factor for the adhesive bonds of soft polymeric materials. The surface profile and roughness of substrates influence the bond strength. Mechanical roughening increases the surface area for effective bonding and removes contaminants from the substrate surface. Therefore, the abrasion process has been widely used as substrate surface pretreatment in various fields of industry.

The profile characteristics of abraded surfaces interrelate with the strength of adhesive joints [1]. Therefore, quantitative estimation of this relation is important. However, at the first it is necessary to investigate profile characteristics of abraded surface by describing a profile of rough surface by some models.

The surface profile produced by roughening using abrasive paper usually is irregular, because grains in abrasive paper are randomly distributed and they are of different size and shape. Therefore, the profile of abraded surface is treated commonly as a realization of random process, which satisfies the assumptions of stacionarity, ergodicity and normality [2, 3]. It is a way to investigate the characteristics of rough surface profile as statistical characteristics. These assumptions are not always satisfied. Therefore, the new models for describing surface roughness have to be created.

Many important spatial patterns of nature are either irregular or fragmented and it is impossible to describe their form by classical geometry. On the other hand, they are nicely described in terms of the concepts of a fractal geometry [4]. These forms often present statistical scale invariance and can be characterized by few parameters like fractal dimensions and scaling exponents [5]. Self-similar fractals are invariant under isotropic length scale transformation – all the different directions scale in the same way. Real surfaces are partially fractal, so they can be characterized, approximated or modeled as having irregular or chaotic geometric components over some range of observation scales.

The aim of this investigation was to find out description of the profiles of abraded surface of soft polymeric materials by fractal model.

2. THEORY

2.1. Fractals

Fractals. Most of man made objects are geometrically simple and can be classified as composition of regular geometric shapes such as lines, curves, planes, circles, etc. Precisely the regular geometric shapes do not approximate some objects. One category of these objects is so called fractals (from Latin *fractus*, meaning irregular or fragmented). Fractals have two interesting characteristics. At the first, fractals are *self-similar* on multiple scales, where a small portion of a fractal often looks similar to the whole object. On the other hand, fractals have a *fractal dimension*, as opposite to integer dimension of the regular geometrical objects. Because fractals are self similar they are constructed by recursion. Typical example is so called Koch curve shown in Fig. 1 [5].

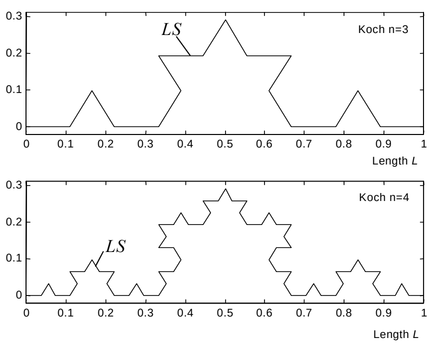

Fig. 1. Koch curve (In each step of construction the middle portion of each segment is removed and replaced by two new line segments. The first step is line, with length $L = 1$) [5]

The interesting parameter of the Koch curve is its length LK. LK is the sum of lengths of segments LS. In the

*Corresponding author: Tel.: +370-37-451658; fax: +370-37-456472.
E-mail address: *loreta.macenaite@ktu.lt* (L. Mačėnaitė)

n-th step length of segment is equal to $LS = 1/3^n$ and the curve consists of 4^n segments. Therefore, $LK = (4/3)^n$. This value increases without bound; hence the Koch curve has infinite length. However, the curve still bounds a finite area.

For stochastic or random fractals the recursion is less explicit than for self-similar fractals and may be an artifact of an underlying fractal building process that occurs on multiple spatial scales. These fractals are called the *self-affine* fractals. In general terms, self-affine fractals have different scaling properties in different directions.

"Box counting" method. The main characteristic of both fractal types is fractal dimension. A variety of different practical approaches to the measurement of the fractal dimension of self-similar structures have been developed and evaluated in [6]. One of the simplest methods used to characterize fractals is known as "box counting". According to this, the fractal lying in a d – dimensional space is covered by a d – dimensional grid with elements of size (length scale) l. The box counting or capacity dimension is then given by

$$D_B = -\lim_{l \to 0}\left(\frac{\log(N(l))}{\log(l)}\right) = \lim_{l \to 0}\left(\frac{\log(N(l))}{\log(1/l)}\right), \quad (1)$$

where $N(l)$ is the number of elements of size l needed to cover a fractal curve. In practice, it is not possible to reach the limit $l \to 0$, so D_B is estimated by measuring the dependence of $\log(N(l))$ on $\log(l)$. D for fractals is not integer.

For the Koch curve it is in the n-th stage $l = LS = 1/3^n$ and $N(l) = LK/LS = 4^n$. Then $D = \log(4)/\log(3) = 1.2619$. The fractal dimension of Koch curve is therefore slightly complex in comparison with the line. For random fractals is simpler to use power spectral density or related functions.

2.2. The statistical surface roughness parameters

Roughness includes the finest (shortest wavelength) irregularities of the surface. Roughness generally results from a particular production process or material condition.

Mathematically profile is the line of section of a surface with a crossing plane, which is (ordinarily) perpendicular to the surface. It is a 2D slice of the 3D surface.

It is possible to evaluate a lot of roughness parameters from a profile of the surface. Classical roughness parameters are based on a set of points $y(x_i)$, ($i = 1, \ldots, N$) defined in the sample length interval L. A set of parameters for profile and surface characterization are collected in [7]. Roughness parameters, which are used, are as follows:

1) Arithmetic average height R_a, also known as the center average line, is the most usually used roughness parameter for general quality control. It is defined as the average absolute deviation of the roughness irregularities from the mean line over one sampling length. This parameter is easy to define, easy to measure. Besides it gives a good general description of the height variation.

The mathematical definition and the numerical representation of the arithmetic average height parameter are, respectively, as follows:

$$R_a = \frac{1}{L}\int_0^L |y(x)|\,dx, \quad (2)$$

$$R_a = \frac{1}{N}\sum_{i=1}^{N} |y_i|. \quad (3)$$

where $y(x)$ is the function, which describes a profile; y_i is the height of a profile at i point, and N is the number of digitized points y_i in a profile.

2) Root mean square (RMS) roughness is R_q. It represents the standard deviation of the distribution of surface roughness heights, so it is an important parameter to describe the surface roughness by statistical methods. This parameter is more sensitive than the arithmetic average height R_a to large deviation from the mean line.

The mathematical definition and the numerical representation of this parameter are as follows:

$$R_q = \sqrt{\frac{1}{L}\int_0^L (y(x))^2\,dx}, \quad (4)$$

$$R_q = \sqrt{\frac{1}{N}\sum_{i=1}^{N} {y_i}^2}. \quad (5)$$

3) Autocorrelation function is ACF. The ACF describes the general dependence of the data values at one position to their values at the other position. It is considered a very useful tool for processing signals because it provides basic information about the relation between the wavelength and the amplitude properties of the surface. The ACF can be considered as a quantitative measure of the similarity between a laterally shifted and an unshifted version of the profile.

The mathematical definition and the numerical representation of this function are as follows:

$$ACF(\Delta x) = \frac{1}{L}\int_0^L y(x)\,y(x+\Delta x)\,dx, \quad (6)$$

$$ACF(\Delta x) = \frac{1}{N-1}\sum_{i=1}^{N} y_i y_{i+1}, \quad (7)$$

where Δx is the shift distance and y_i is the height of the profile at i point. ACF can be normalized to have a value of unity at a shift distance of zero. This suppresses any amplitude information in ACF but allows a better comparison of the wavelength information in various profiles.

3. EXPERIMENTAL

Some forms of mechanical treatments improve the strength of bonds by removing the contaminants from the surface as well as increasing the size of bonding area. We have studied roughness of soft polymeric materials, because surface roughness is the important design factor for the adhesive bonds.

As substrate for investigation monolithic butadiene-styrene rubber was selected. The density and hardness according Shore A of BSR rubber was $\rho = 1.25$ g/cm^3 and $H = 75$ Sh A, respectively.

The rubber surface roughening was performed on the abrasion machine, which contains special device for applying constant pressing force between specimen and abrasion disk.

Five different grades of abrasive paper (*N* 24, *N* 36, *N* 40, *N* 60, *N* 100) were used to produce different degrees of roughness on the rubber surface.

Surface roughness of the abraded rubber was tested by Hommelwerke *T*500 surface finish tester – profilograph (Germany). The profile of abraded surface was carried out perpendicular to the abrasion direction. The typical view of profiles is presented in Fig. 2.

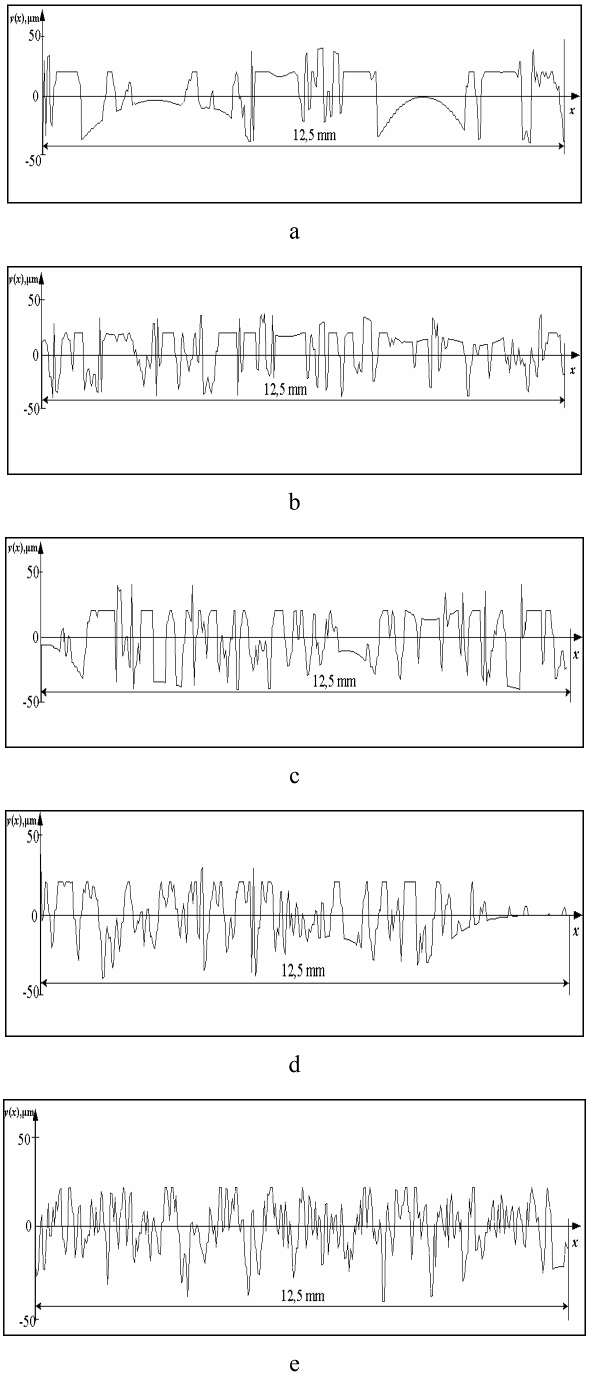

Fig. 2. The profiles of rubber surface abraded by different grade of abrasive paper: *a* – *N* 24; *b* – *N* 36; *c* – *N* 40; *d* – *N* 60; *e* – *N* 100

4. RESULTS AND DISCUSION

4.1. The profile of surface roughness

The degrees of surface roughness produced by treatment with abrasive paper of different grades in terms of the R_a and R_q are presented in Table 1.

Table 1. Statistical parameters of surface roughness of rubber produced by five different grades of abrasive paper

Grade of abrasive paper	Statistical parameters	
	R_a (μm)	R_q (μm)
N 24	18.932	19.756
N 36	18.616	18.840
N 40	16.514	18.101
N 60	11.030	16.115
N 100	10.018	10.825

It is demonstrated that decreasing of grade of abrasive paper increases R_a value. Fig. 2 shows the irregular profiles produced by roughening the surface of the rubber.

In this paper the high frequency (or short wave) components of surface profile is referred to the surface roughness. According to this definition of roughness a profile of rubber surface abraded by abrasive paper *N* 100 is rougher than a profile of rubber surface abraded by abrasive paper *N* 24.

The profiles of abraded rubber surface satisfied the assumptions of stacionarity, ergodicity and normality [3]. Therefore, geometric structure of abraded surface profile can be treated as a realization of random process.

4.2. Surface roughness and fractal dimension

A convenient characteristic of isotropic surfaces smoothness is fractal dimension. The data of surface roughness profile represents curve in plane. Two dimensional fractal dimension *D* of surface profile is the number between 1 (for smooth curve) and 2 (for rough curve) [5, 6]. This assumption was checked for roughness of soft polymeric materials surface.

The fractal dimensions of surface profiles of roughened rubber have been evaluated by “box-counting” method according to Eq.(1). The fractal dimensions of rubber surface profiles produced by treatment with five abrasive paper of different grades are presented in Table 2.

Table 2. Estimation of fractal dimension

Grade of abrasive paper	R_a value (μm)	Fractal dimension *D*
N 24	18.932	1.3856
N 36	18.616	1.4972
N 40	16.514	1.5359
N 60	11.030	1.6611
N 100	10.018	1.7925

Table 2 demonstrates that fractal dimension D increases as R_a decreases. One we can seen, the obtained results satisfied the assumption that increase of rubber surface roughness fractal dimension D increases.

It was determined that the empirical relationship between R_a and D is fitted to model

$$R_a = \frac{1}{0.1340D - 0.1395}. \tag{8}$$

This model explains 90.26 % of the variability in R_a. The fitted model is shown in Fig. 3. The correlation coefficient is equal to 0.950047 and it indicates a strong relationship between the variables R_a and D.

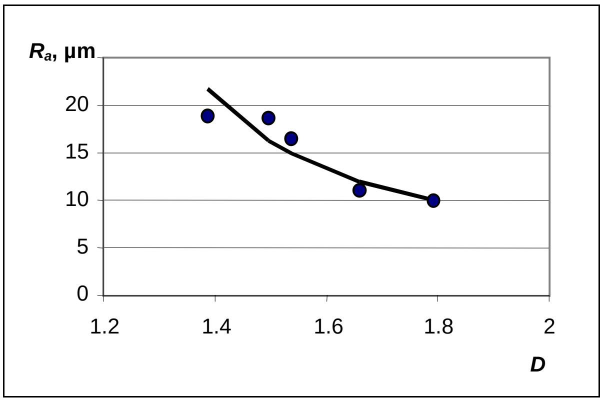

Fig. 3. The empirical relationship between R_a and D: smooth curve corresponds to fitted model (Eq.(8))

The empirical relationship between R_q and D was described, also. The equation of fitted model is

$$R_q = 50.8587 - 21.6781 \cdot D. \tag{9}$$

This linear model explains 90.93 % of the variability in R_q. The fitted model is shown in Fig. 4. The correlation coefficient is equal to –0.9535 and it indicates a strong relationship between the variables R_q and D.

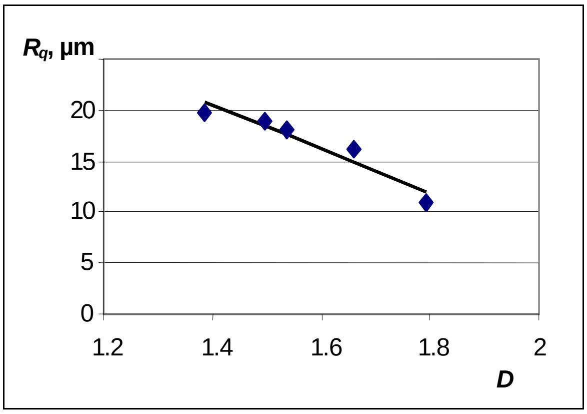

Fig. 4. The empirical relationship between R_a and D: smooth curve corresponds to fitted model (Eq.(9))

Roughness includes the short wave (high frequencies) irregularities of the surface. It was shown that statistical parameter R_q is the function of fractal dimension and cut-off frequencies only [8]. The term "cut-off" numerically specifies the frequency bound below or above which the components of roughness are extracted or eliminated. R_q can be expressed as:

$$R_q = \frac{G^{2(D-1)}}{4-2D}\left(\frac{1}{\omega_l^{(4-2D)}} - \frac{1}{\omega_h^{(4-2D)}}\right), \tag{10}$$

where ω_l is the lower wave number limit and ω_h is the higher wave number limit. They are related to the length of sample L and sampling interval Δx respectively:

$$\omega_l = \frac{\pi}{L}, \ \omega_h = \frac{\pi}{\Delta x}. \tag{11}$$

Roughness parameter R_q depends on the properties of a surface and varies in depending on the conditions of measurement.

The parameter R_q of roughened rubber surface according to Eq.(5), Eq.(9) and Eq.(10) was calculated. The obtained results are presented in Table 3.

Table 3. Estimation of root mean square roughness R_q

Grade of abrasive paper	R_q (μm) (Eq.(5))	R_q (μm) (Eq.(9))	R_q (μm) (Eq.(10))
N 24	19.756	20.822	20.541
N 36	18.840	18.402	19.375
N 40	18.101	17.563	17.353
N 60	16.115	14.849	17.246
N 100	10.825	12.001	15.120

4.3. Simulation of surface roughness

Some models of rubber surface profile was analyzed in previous works [9, 10]. The surface profile was approximated according to cubic splines and Fourier series. These models describe a surface profile of roughened rubber very well but it is a problem to employ these models in practical computation. Therefore, new models for describing surface roughness are searched.

Fractal geometry has been proposed as a mean to characterize surface roughness [5, 11, 12].

Self–affine curves are commonly used to describe the surface roughness [5, 6, 13]. The Weierstrass - Mandelbrot function (*W–M* function), satisfying to the self-affinity requirement is most widely used by generating self-affine curves. It can be expressed as:

$$y(x) = G^{D-1}\sum_{i=n_1}^{\infty}\frac{\cos(2\pi\gamma^i x)}{\gamma^{i*(2-D)}}, \tag{12}$$

where $y(x)$ is the height of surface in the point x; $1 < D < 2$ is fractal dimension, G is characteristic length scale of surface and γ^i determines the frequency spectrum of surface roughness. It was determined that the value of this parameter is $\gamma = 1.5$. The lowest frequency is then related to the sample length L according to the relation

$$\gamma^{n_1} = 1/L. \tag{13}$$

The evaluation of D and G from random fractals is based on the power spectral density function $P(\omega)$, which is expressed as follows:

$$P(\omega) = C \cdot \omega^{-B}, \tag{14}$$

where $C = \dfrac{G^{2(D-1)}}{2\ln(\gamma)}$, $B = 5 - 2D,$ when $1/L \le \omega \le \infty$.

The power spectral density function $P(\omega)$ has power law of the form, which is typical feature of fractals.

The profiles of surface of roughened rubber have been generated by *W–M* function. The autocorrelation functions of real and simulated profilogramms were chosen as the criterion of equivalence of real and simulated profiles.

The empirical autocorrelations functions of rubber surface profiles produced by treatment with five different grades of abrasive paper were compared with the empirical autocorrelation functions of profiles simulated by *W–M* function. Two typical normalized autocorrelation functions are shown in Fig. 5.

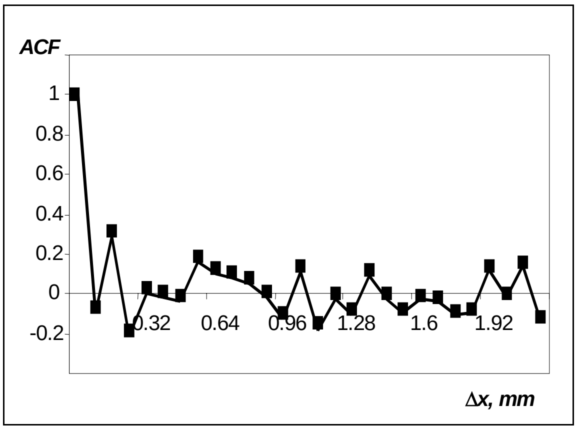

Fig. 5. The empirical autocorrelation functions (Markers ■ correspond to autocorrelation function of real profile; smooth curve corresponds to autocorrelation function of profile generated by *W–M* function)

This Figure shows that they are practically identical. Therefore, it has been concluded that a rubber surface roughness can be generated by *W–M* function.

CONCLUSIONS

According to our simulations the surface of abraded rubber can be modeled by *W–M* function.

The results show that fractal dimension *D* determines the degree of rubber surface roughness. The profile of surface roughness has the fractal dimension *D* between 1 (for smooth profile) and 2 (for rough profile).

Relations between fractal dimension *D* and statistical parameters (R_a, R_q) have been determined. Thus, some characteristics of surface roughness can be calculated by using fractal dimension only.

REFERENCES

1. **Niem, P., Lau, T., Kwan, K.** The Effect of Surface Characteristics of Polymeric Materials on the Strength of Bonded Joints *J. Adhesion Sci. Technol.* 10 (4) 1996: p. 361 – 372.
2. **Chusu, A. P., Vitenberg, J. R., Palmov, V. A.** Roughness of Surfaces, Moscow, 1975 (in Russian).
3. **Petraitiene, S., Brazdziunas, R., Pekarskas, V.** The Statistical Characteristics and Their Interrelation of Abrasives and Surface Coarse After the Process with Them *Materials Science* (*Medžiagotyra*) 1997 1 (4) pp. 44 – 46.
4. **Mandelbrot, B. B.** The Fractal Geometry of Nature. Freeman, San Francisco, 1982.
5. **Feder, J.** Fractals. Moscow, 1991: 260 p. (in Russian).
6. Fractals in Physics (Ed. by L. Pietronero and E. Tosatti). Moscow, 1988 (in Russian).
7. **Gadelmawla, E.S., Koura, M. M., Maksoud, T. M., Elewa, I. M., Soliman, H. H.** Roughness Parameters. *Journal of Materials Processing Technology* 123 (2002) pp. 133-145.
8. **Wu, J. J.** Characterization of Fractal Surfaces *Wear* 239 2000: pp. 36 – 47.
9. **Macenaite, L., Pekarskas, V.** Approximation of Profilogramms of the Surfaces of Soft Polymeric Materials *Product Technologies and Design. Materials of Conference Presentations,* Kaunas: Technology, 2000: pp.48 – 52 (in Lithuanian).
10. **Macenaite, L., Pekarskas, V.** Analysis of Correlation Functions for Surface Profilogramms of Polymeric Materials *Product Technologies and Design: Materials of Conferences Presentations,* Kaunas: Technology, 2002 (in Lithuanian).
11. **Majumdar, A., Tien, C. L.** Fractal Characterization and Simulation of Rough Surface *Wear* 136 1990: pp. 313 – 327.
12. **Majumdar, A., Bhushan, B.**. Role of Fractal Geometry in Roughness Characterization and Contact Mechanics of Surfaces *Journal of Tribology, Transactions of the ASME* 112 1990: pp. 205 – 216.
13. **Ganti, S., Bhushan, G.** Generalized Fractal Analysis and Its Applications to Engineering Surfaces *Wear* 180 1995: pp. 17 – 34.

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