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The Modeling of Soft Polymer Materials Surface Profiles

Loreta MAČĖNAITĖ*, **Kristina MASILIONIENĖ**, **Vidmantas PEKARSKAS**

Faculty of Fundamental Sciences, Kaunas University of Technology, Studentų 50, LT-51368 Kaunas, Lithuania

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The results of roughened rubber surface profilogramms approximation by cubic splines and Fourier series and its modelling by Monte Carlo method are presented. As a main parameter of profile, an autocorrelation function was selected. It was shown that the profile of surface roughness in dependence of abrasion paper grade number and experimental procedures can be predicted theoretically.
Keywords: abrasion, surface roughness, autocorrelation function.

INTRODUCTION

The strength of adhesive joints is in high dependence on the real contact surface area, i. e. on the surface roughness of substrate [1 – 3]. Usually, surface roughness is increased by abrasion with different grade number paper. The obtained surface roughness is investigated by caring out profilogramms. Mathematically, the profile of abraded surface is commonly treated as a realization of random process. According to the earlier obtained results of the statistical investigation of roughened rubber surface, it was determined, that it can be approached as a realization of stationary normal process [4]. In this case, one of the main surface roughness statistical parameters is autocorrelation function of profile [5]. In order to calculate autocorrelation function values, profile previously must be discretized and numerically evaluated. Only after that two-dimensional data array, which is used for calculation values of autocorrelation function, is composed [6].

As the profiles of rubber surface contain complex structure, it is difficult to evaluate and calculate real profile length of contact. In this case more pronounced way is to approximate profile length by means of more simple function relations.

The aim of this investigation was to approximate and to model profiles of soft polymer materials surface in dependence on the grade number of abrasive paper used for surface roughening.

EXPERIMENTAL

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

To produce roughness on the rubber surface abrasive paper grade number N of 24, 36, 40, 60 and 100 was used. Grade number N of abrasive paper is a relative value, which increase indicates the decrease of abrasive particle size. Practically, the increase of grade number N of abrasive paper results on the increase of the surface smoothness after abrasion.

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

The profiles from roughened surface were carried out perpendicular to the abrasion direction using the surface finish tester-profilograph Hommelwerke T500 (Germany).

RESULTS AND DISCUSSION

The profile of surface roughness in the sample length interval l is expressed as a set of M points with coordinates (x_i, $y(x_i)$) defined. The sample length l is equal 12.5 mm. The typical view of profiles obtained after surface abrasion with different grade number paper is presented in Fig. 1.

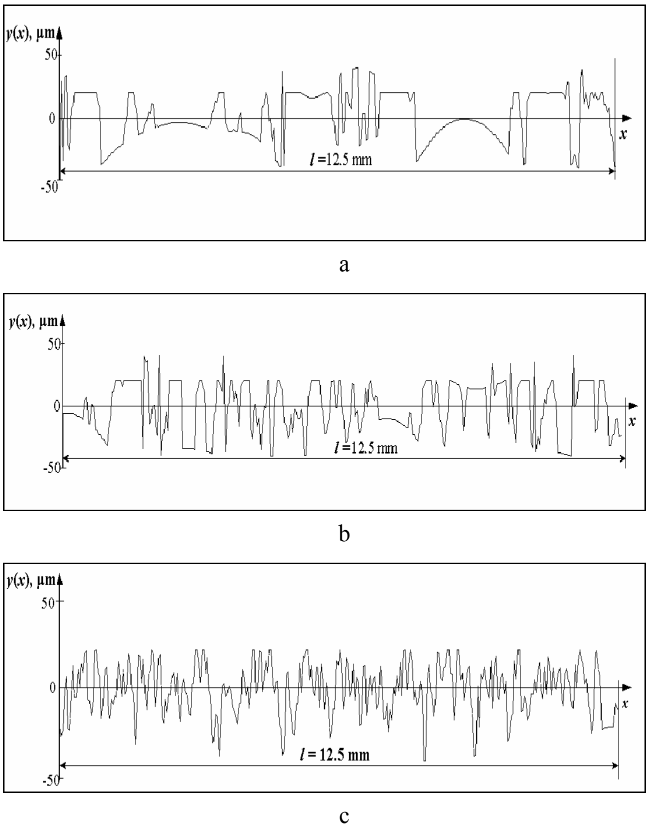


Fig. 1. The typical profiles of abraded rubber surface in dependence of abrasive paper grade number N: a – 24, b – 40, c – 100

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

Determination of profilogramms autocorrelation functions (*ACF*). The autocorrelation function $ACF(\tau)$ describes the general dependence of correlation coefficient between the data values at one position to their values moved to the other position by step τ. The mathematical definition and numerical representation of this function are as follows [7]:

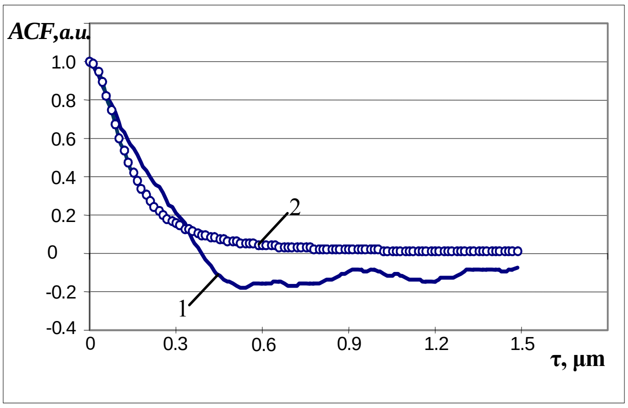
$$ACF(\tau)=\frac{1}{l}\int_0^l y(x)y(x+\tau)dx\,; \tag{1}$$

$$ACF(\tau)=\frac{1}{M-1}\sum_{i=1}^{M} y_i y_{i+1}\,. \tag{2}$$

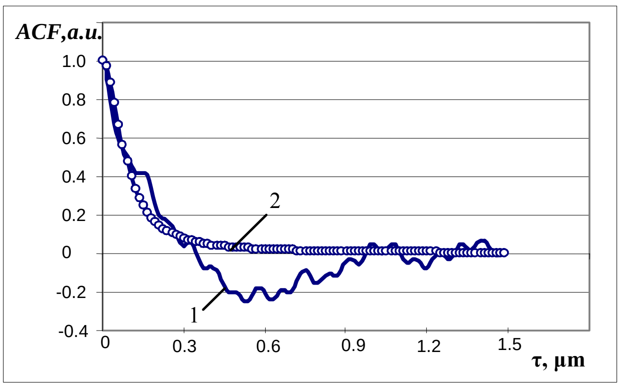
where $y(x)$ is the function, which describes a profile; y_i is the height of a profile at i point, M is the number of digitized points in length interval l, $\tau=x_{i+1}-x_i$ is a size of discretization step, l is the sample length interval.

As each realization can strongly differ from other, all the obtained rubber profile after abrasion with the same grade paper number were firstly discretized, averaged and only then autocorrelation function was constructed. *ACF* was normalized in order to obtain a value of 1 at a shift distance of zero.

Fig. 2 shows autocorrelation function of real rubber surfaces profiles, obtained after surface roughening with abrasive paper which grade number of $N = 40$ and $N = 100$.



a



b

Fig. 2. The empirical autocorrelation function (1) and approximation function (2) for roughened rubber surface in dependence on the abrasion paper grade number *N*: *a* – 40, *b* – 100

Assuming that an analytical expression of empirical autocorrelation function must coincide with the real autocorrelation function and must be convenient for calculations, such type of autocorrelation function was selected:

$$ACF(\tau)=\frac{1}{1+(\alpha\tau)^2}\,, \tag{3}$$

where α is the parameter determined by least square method and it depends on the abrasion paper grade number N. [8]

The autocorrelation functions approximated according to the Eq. 3 are presented in Fig. 3.

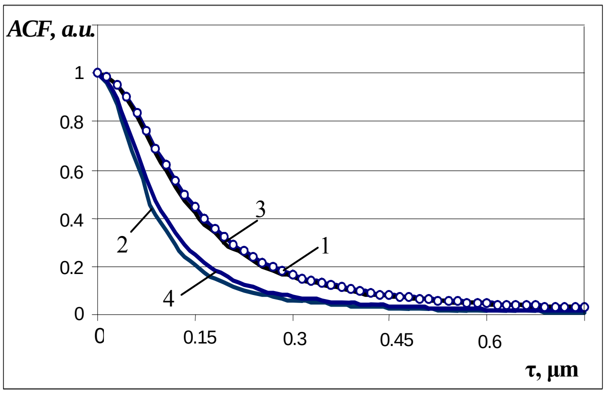


Fig. 3. The autocorrelation functions of roughened rubber surface in dependence on the abrasion paper grade number *N*: 1 – 24, 2 – 60, 3 – 40, 4 – 100

The approximation profiles by cubic splines and Fourier series. The autocorrelation function can be used for checking randomness of data set, too [7]. If data are random, then correlation coefficients values should be near zero for all discretization step τ. If data are non - random, then one or more of the correlation coefficients values will be significantly and not equal to zero.

In this work determined empirical autocorrelation functions show that the profile of surface roughness is not random, but rather has high degree of correlation between adjacent values. That indicates that rubber surface profiles can be expressed and analyzed as mathematical models.

As can be seen from the previously presented data, the profiles of roughened rubber surface are curves of complex structure. Due to that it is impossible to approximate it according to the function expressed by one analytical equation. It was determined, that the roughened surface of soft polymer material it is purposeful approximate by cubic spline interpolation and Fourier series [9].

The cubic spline interpolation is a piecewise cubic polynomial, which is 2 times continuously differentiable. In cubic spline interpolation cubic polynomials:

$$S_i(x)=A_i(x-x_i)^3+B_i(x-x_i)^2+C_i(x-x_i)+D_i \tag{4}$$

are used on each interval $[x_i, x_{i+1}]$, $i=\overline{0,M}$. The cubic polynomials coefficients A_i, B_i, C_i, D_i are evaluated for each interval $[x_i, x_{i+1}]$. For the profiles interpolation discreet points were selected in such way, that characteristic distance between them was equal to the $\Delta x = 0.08$ mm.

The next model of rubber surface roughness profiles approximation was Fourier series [9 – 12].

Fourier series describe the profile height function $y(x)$ as shown below:

$$y(x)=\frac{a_0}{2}+\sum_{n=1}^{\infty}\left(a_n\cos n\omega_0 x+b_n\sin n\omega_0 x\right), \quad (5)$$

where $\omega_0=\frac{2\pi}{l}$ is the fundamental frequency. The coefficients a_0, a_n, b_n are calculated according to the following equations:

$$a_0=\frac{1}{l}\int_{-\frac{l}{2}}^{\frac{l}{2}}y(x)dx\,; \quad (6)$$

$$a_n=\frac{2}{l}\int_{-\frac{l}{2}}^{\frac{l}{2}}y(x)\cos n\omega_0 x dx\,; \quad (7)$$

$$b_n=\frac{2}{l}\int_{-\frac{l}{2}}^{\frac{l}{2}}y(x)\sin n\omega_0 x dx\,. \quad (8)$$

In order to evaluate the accuracy of approximation by means of Fourier series, the empirical autocorrelation functions, representing real profile length and those approximated by selected method were compared. The typical result is presented in Fig. 4.

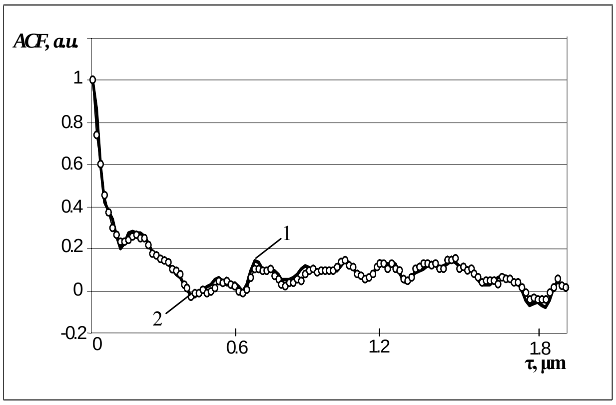


Fig. 4. The empirical autocorrelation function of real profiles (1) and those approximated by Fourier series (2)

The difference between profiles approximated by cubic splines, Fourier series and real profiles autocorrelation function is negligible: 16 from 25 profiles approximated by cubic splines, autocorrelation coefficients and those 15 from 25 profiles, approximated by Fourier series are statistically important at the 95 % of confidence level. These results indicate that both of selected models coincide well with the real profile of abraded rubber surface.

The modelling of profiles by Monte Carlo method. The possibility to create profile model by method of Monte Carlo has been investigated, also. This method is based on the random generation of ordinate values of profile points [13, 14]. The selected type of modelling was based on the Eq. 3 using the algorithm expressed according to the relation:

$$\xi[n]=\sum_{k=1}^{N}c_k x[n-k], \quad (9)$$

where $\xi[n]$ is the modelled random value; $x[n]$ are independent, normally distributed random values, average of which is equal to 0 and dispersion is equal to 1; c_k are the validity coefficients; N is the number of modelled process values; n is the integer-valued parameter. The validity coefficients c_k values were calculated according to the formula:

$$c_k=\frac{1}{\omega_c}\int_0^{\omega_c}\left(\frac{\omega_c}{\pi}G(\omega)\right)^{\frac{1}{2}}\cos\frac{k\pi\omega}{\omega_c}d\omega\,, \quad (10)$$

where $\omega_c=\frac{\pi}{\tau}$, $G(\omega)$ is the spectral density of modelled process, when $-\omega_c\le\omega\le\omega_c$ is the frequency range.

If autocorrelation function is expressed according to the Eq. 3, then:

$$c_k=2\sigma\sqrt{\frac{\gamma}{\pi}}\cdot\frac{1}{1+4\gamma^2k^2}\,, \quad (11)$$

where σ is the standard deviation of modelled process; $\gamma=\alpha\cdot\tau$ is the dimensionless parameter ($\gamma\le\frac{1}{2}$).

The accuracy of created model was evaluated by comparison of autocorrelation function determined using Eq. 3 and autocorrelation functions of both real and modelled processes. The results of this comparison are presented in Fig. 5.

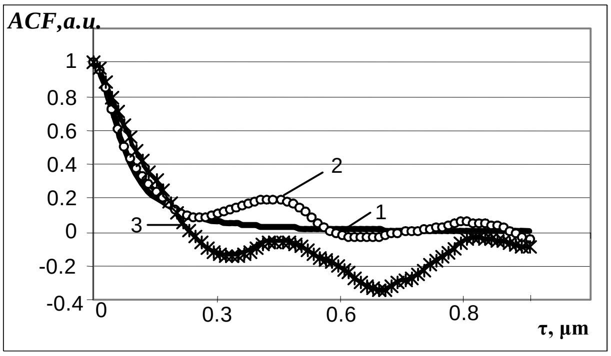


Fig. 5. The comparison of approximated (1), modelled (2) and real (3) autocorrelation functions of roughened rubber surface profiles (grade number $N = 36$)

The influence of autocorrelation function (Eq. 3) parameter α in dependence on the abrasion paper grade number N, which was used for rubber surface roughening, has been determined, also. After 4-th order polynomial approximation of the results, the following analytical expression was determined:

$$\alpha=-1{,}1939\cdot10^{-6}N^4+0{,}2654\cdot10^{-4}N^3-\\-0{,}0202\cdot N^2+0{,}6263N-6{,}5652. \quad (12)$$

The obtained results are presented in Fig. 6.

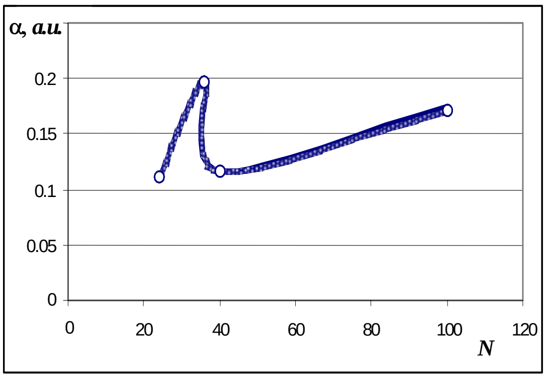


Fig. 6. The influence of abrasion paper grade number N on the parameter α

The Eq. 12 allows to calculate parameter α values in dependence on the abrasion paper grade number. Besides, roughness of rubber surface can be calculated for paper grade number, which has not been realized during experimental procedure. This method allows also to model the surface roughness profile without real profile data.

The suitability of this method shows results of control experimental data, by carring out profiles from rubber surface, roughened with abrasive paper, which grade number was $N = 60$. In Fig. 7 two autocorrelation functions are presented: one of them was carried out from the real surface and another one modelled by method of Monte Carlo. The modelling of this profile was based on the autocorrelation function approximation according to the Eq. 3. The value of parameter α was calculated according to the Eq. 11, when $N = 60$.

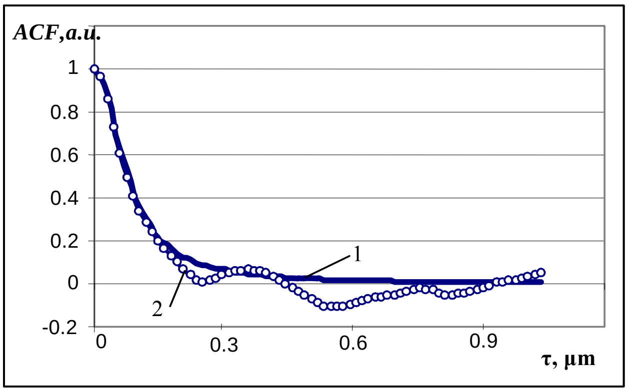


Fig.7. The comparison of prediction and control results: 1 – the autocorrelation function of real profiles, 2 – the predicted autocorrelation function

So, results presented in Fig. 7 show that there are no difference between models when the step is not higher than 0.15 and only insignificant differences were found at bigger step τ values.

CONCLUSIONS

It was determined that profiles carried out of roughened by abrasion soft polymer materials surface can be approximated by cubic splines and Fourier series.

Profiles of soft polymer materials can be modelled by method of Monte Carlo, also.

The obtained results allow to predict profile of surface roughness in dependence of abrasion paper grade number without experimental procedures.

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