Modeling of geometric and optical properties of textured polymer coatings of steel sheet with anisotropic defects

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Abstract. The study of the surface of sheet metal with polymer coatings by optical microscopy method showed that it consists of grooves which collect in star-like condensations on the surface. When comparing images obtained by an optical microscope and the method of scanning probe microscopy, we observed scale invariance. Therefore, the distribution of defects on the surfaces of the polymer coatings of the metal sheet is neither deterministic nor purely random, and so this distribution is fractal in nature. To study geometric and optical properties of textured coatings, we used a three-dimensional anisotropic model based on the Julia set. We developed the method which allows determining the values of the parameters of this model for a number of samples of coatings of steel sheet obtained under different conditions of their formation. The fractal dimension of objects obtained on the base of this model is determined. The scattering of electromagnetic waves from the surface of polymer coatings was studied by means of the Kirchhoff method.

1. Introduction

The solution of the problem of creating surfaces with certain properties is necessary both for their stable functioning of products so for technological control of the surface quality of such products [1]. The use of the fractal approach to describe structural inhomogeneities, as well as the justification of general regularities, is one of the modern scientific trends in surface physics and chemistry of solids. At present, various mathematical models of fractals (Sierpinski rug, Mandelbrot set), describe well the real imperfections (Brownian) surfaces of metal layers, dielectric layers [2], semiconductor surfaces [3] that have defects of a symmetric type [4, 5]. However, when examining the surface of polymer coatings of a metal sheet, the detected defects are anisotropic; therefore these models cannot be used to describe their structure. In this paper, a three-dimensional anisotropic model based on the Julia set was used to construct a fractal model of the surface.

2. Algorithm of building fractals

To construct fractal surfaces of textured polymer coatings of sheet metal (figures 1a, b), the following algorithm was used:

1. The area in which the fractal is created is divided into 1000x1000 rectangles. Each rectangle is characterized by the coordinates \((X_{r,s}, Y_{r,s})\) of its center

2. A sequence is defined by the recurrence formula [6]
\[ Z^{(n)}_{r,s} = \left( Z^{(n-1)}_{r,s} \right)^2 + p + iq, \]  \hfill (1)

where values \( p \) and \( q \) are parameters of the fractal function (1). The first point of the sequence is defined as

\[ Z^{(1)}_{r,s} = X_{r,s} + iY_{r,s}. \]

3. The value of \( H \), inverse to the rate of increase of the modulus of the sequence (1) is introduced. \( H \) is equal to the smallest number of the sequence term, when \( |z_i| > Q \). In our calculations, we assumed that the value is \( Q = 10^6 \).

The examples of fractal functions obtained are shown in figures 1c, d.

**Figure 1.** Pictures of samples 1 and 2 obtained by an optical microscope method (a and b) and the fractal models of their surfaces (c and d correspondingly).

3. **Determining the geometrical parameters of fractal functions**

The type of defects (grooves) in textured coatings depends on the conditions of its formation. In figures 1a and 1b, the surface relief images of two samples coated by the same polyester material are shown. The coating of the sample 2 was formed at a higher temperature, which affected the parameters
of the grooves. Table 1 presents the mean parameters of the "grooves" on the surface of the samples 1 and 2. To determine the parameters of the fractal model, \( p \) and \( q \), the constructed fractal functions were compared with the surface images (table 1).

**Table 1.** Parameters of textured coatings measured with an optical microscope and parameters of fractal surfaces.

| №  | Average values of furrows parameters | Model parameters | Scale \( m = L/L_0 \) (\( \mu \text{m} \)) |
|----|-------------------------------------|-----------------|-----------------------------------------|
|    | Width \( d \) (\( \mu \text{m} \)) | Length (\( \mu \text{m} \)) | Height (\( \mu \text{m} \)) | Radius of curvature (\( \mu \text{m} \)) | \( p \) | \( q \) |
| 1  | 34.7                               | 545             | 36.2                                   | 1378                                   | -0.55375 | 0.55008 | 0.945 |
| 2  | 28.5                               | 523             | 31.3                                   | 1371                                   | -0.57125 | 0.55047 | 0.985 |

To determine the magnitude \( m = L/L_0 \), the middle length \( L_0 \) of grooves measuring by an optical microscope method (see figures 1a, b) and the length of the median line of the fractal function \( L \) (see figure 2b) were compared. For this purpose, at the construction of fractals, we used the cubic polynomial approximation (figure 2a) and calculated its length \( L \).

![Figure 2](image_url)

**Figure 2.** The construction of the median line (a). The length of the median line (b), the mean width of the polygon (c) and the average curvature (d) vs. the parameter \( p \) for different values of the parameter \( q \).
The width $d$ is defined by dividing the polygon fractal area and the length $L$. The radius of curvature $R$ is determined as a mean radius of curvature of the median line.

Figure 1c and d show fractal functions for samples 1 and 2, under which the experimental and theoretical parameters coincide. Figures 2c and d show the dependences of the values of $d$ and $R$ on the parameters $p$ and $q$ of the fractal function (1).

The fractal dimension was calculated using the following algorithm:

- A cube is constructed in the three-dimensional $NxM$ space, where $N$ and $M$ are the numbered points of the fractal surface. The size of the cube edge must be a factor of the smallest unit of the fractal surface.
- It is checked, whether the constructed cube locates particularly or fully in the fractal figure.
- If it locates, then the number of cubes is increased by one.
- The neighboring cube is constructed.
- Firstly the bottom level of the surface is filled, and then the next level is filled, etc.
- If at some level, no cube enters in the fractal (the empty space), then the cycle is finished.

The dependence $\ln \left( M_\xi \right)$ on $\ln \xi$ is shown in figure 3. Here $M_\xi$ is the number of cubes entering in the fractal, and $\xi$ is the cube edge. From the slope of this dependence we obtained the fractal dimension $k=2.29$.

![Figure 3](image_url)

**Figure 3.** Determining the dimension of the fractal. The points represent the modelling data; the solid line is the corresponding linear regression.

4. Study of optical properties of textured surfaces.

The scattering of light is associated with a number of structural features of polymers, and it is widely used for their investigation [7-9]. In this paper, it was assumed that light falls on a rough surface $S$ at a given angle of falling light $\theta_1$ and it is scattered in all directions. The scattered wave is characterized by the polar angle $\theta_2$ and the azimuthal angle $\theta_3$ (figure 4). The intensity of light scattered in the direction $(\theta_2, \theta_3)$ is measured by the detector $D$. 


Using the basic formula of the Kirchhoff method, the strength of scattered field is calculated under the following conditions:

- the incident wave is monochromatic and flat;
- the scattering surface is rough inside the rectangle under consideration and smooth beyond the boundaries;
- the size of the rough surface is much larger than the length of the incident wave;
- the scattering field is observed in the wave zone, i.e., far enough from the scattering surface.

To study the scattering of light, we used the formulas given in ref. [9]. The dependence of the reduced intensity of scattered light $I/I_0$ on the angles $\theta_2$ and $\theta_3$ at $\theta_1 = 45^\circ$ for the red light is shown in figure 5. Here $I_0$ is the maximum calculated value for sample 1.

The intensity of the scattered light by the surface of sample 2, formed at a higher temperature, is less by 21%. For experimental verification of the results obtained, the gloss of the samples under study was measured. Experimental studies have shown that at the same angle of incident light, the gloss of sample 2 is 18% less than sample 1. The difference between theoretical and experimental results can be explained by the fact that photometric instruments in studying such textured coatings have a large error due to strong scattering of light on them.

Figure 5. The reduced intensity of scattered light vs. the polar $\theta_2$ and horizontal $\theta_3$ angles for the samples being considered. $\theta_1 = 45^\circ$. 

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5. Conclusion
Surfaces of textured polymer coatings of metal sheet are rough and can change their shape under different conditions of their formation. The physical phenomena occurring on these surfaces cannot be described in terms of the standard deviation of the peak height of the correlation function for them. Real surfaces are most adequately described by fractal functions, that is confirmed by experimental results on the scattering of light. These results can be used to study other physical phenomena on the surfaces described, such as friction, electrical conductivity, and capacity.

6. References
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