Modeling of light scattering by polymer coatings of rolled metal surface

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Abstract. The statistical characteristics of light scattering on textured polymer coatings of rolled metal surface are studied on the base screen model with two-dimensional Weierstrass function. In the frame of the Kirchhoff method, the average light scattering and gloss coefficients are numerically calculated for different coating surface calibration (profiles) and falling angles. It is shown; that the scattering is symmetrical relatively to the plane of incidence and it is maximal in the direction $\theta_1 = 0$. The scattering wave is observed in the cone of lateral directions relatively the normal direction $\theta_2 = 0$. For such coatings it is necessary to develop a special convergence experimental technique allowing identifying a correspondence between the gloss and the texture of the surface.

1. Introduction

Rolled metal with a textured polymer coating must be characterized by high mechanical and optical characteristics, which give the building structures (roofs, etc.) good decorative qualities, namely, a natural and noble appearance typical for the structure and color of natural tiles. The mechanical properties (the strength, durability and etc.) of the branded products “Steel Velvet” and “Steel Silk” of PAS “Severstal” (Cherepovets) correspond to parameters required by world standards [1, 2]. However, photometric instruments underestimate the gloss coefficient and total deviation of the color coordinates of the sample from the corresponding optical properties of the standard. At present, the comparison of optical characteristics (the gloss, color etc.) of textured polymer coatings with the corresponding ones of standard occurs often visually (“by eye”), without the use of magnifying and special optical devices. Therefore, it’s necessary to find out the reasons for this discrepancy. For this purpose, preliminary, we studied experimentally the sample surface of a textured polymer coating using scanning probe microscopy method. As can be seen from Fig. 1, the surface of textured coating has a rough fractal character. Therefore, we supposed that one from reasons for this discrepancy is the significant light scattering on the by randomly rough surface of the coating.

In this paper the average coefficient of light scattering and the gloss coefficient are calculated in the frame of the Kirchhoff method. A normalized Weierstrass function is used for modeling 2D fractal rough surface. The analogues calculations of scattering indicatrices diagrams for various surfaces and incidence angles were performed by others authors [3-7], but our results have some distinctive features, related with calculation of the gloss coefficient.

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Figure 1. The sample of steel sheet with 200-fold magnification with the probe attached to it.

Figure 2. The example of a rough fractal surface simulated by means of the Eq.(1) at $N = 10, M = 10, D = 2.5, q = 2, K = 3$.

2. Fractal-like model for two-dimensional rough surfaces

Usually [4,5], for the simulation of rough surfaces, the modified two-dimensional Weierstrass function $z(x,y)$ for the height of roughness is chosen. This function has the form:

$$z(x,y) = c_w \sum_{n=0}^{N-1} \sum_{m=1}^{M} q^{(D-3)n} \sin \left\{ K q^n \left[ \frac{2 \pi n}{M} x \cos \frac{2 \pi m}{M} + y \sin \frac{2 \pi m}{M} \right] + \varphi_{nm} \right\},$$

where $c_w$ is a normalizing constant. The number $K$ determines the wave length of the surface’s fundamental harmonic. The value $q$ characterizes both the amplitude and frequency of harmonics ($q > 1$). The numbers $N, M, D$ and $q$ determine the surface calibration degree because of imposing additional harmonics on the fundamental wave, and $N$ and $M$ determine the number of overtones. The number $D$ is the fractal dimension that determines the amplitude of harmonics (usually $2 < D < 3$).

It was shown [4-6] that the large scale spatial heterogeneity of the surface increases, too with an increase in $N, M, D$ and $q$.

The phases $\varphi_{nm}$ in Eq. (1) can be chosen in appointed or casual ways, what gives deterministic or stochastic function $z(x,y)$, respectively. As the rule [3-7], the functions $\varphi_{nm}$ are considered as casual values distributed uniformly over the interval $[-\pi, \pi]$. Particular realization of the function $z(x,y)$ with the parameters $c_w$, $q$, $K$, $D$, $N$, $M$ chosen beforehand can be received with each particular choice of numerical values of all $N \times M$ phases $\varphi_{nm}$ with the help of a random-number generator. Therefore, the function determined by Eq. (1) is a combination of determinate periodic and random constituents. This function may be anisotropic in both directions, given $M$ and $N$ are not too large. Since natural surfaces are generally neither purely random nor purely periodic, and often anisotropic, this function proposed is a good candidate for modeling natural surfaces [3-7].

The example of a rough surface simulated by means of the equation (1) is shown on Figure 2.

Every possible realization of the function $z(x,y)$ forms an ensemble of surfaces. Deflection of the rough surface points from the basic plane appears to be proportional to the value $c_w$; therefore, this parameter is connected with the height of structure imperfections over the surface. It is found more convenient to set a rough surface by choosing the root-mean-square height of its profile $\sigma$ which can be calculated using the expression:

$$\sigma \equiv \sqrt{\langle h^2 \rangle}$$
where \( h = z(x,y) \), the notation \( \langle \cdots \rangle \geq \prod_{n=0}^{N-1} \prod_{m=1}^{M-1} \int_{-\pi}^{\pi} \frac{d\phi_{nm}}{2\pi} \ldots \) means ensemble averaging over the surfaces. The relation between the parameters \( c_w \) and \( \sigma \) can be established taking the integrals directly:

\[
\sigma = \left[ \prod_{n=0}^{N-1} \prod_{m=1}^{M-1} \int_{-\pi}^{\pi} \frac{d\phi_{nm}}{2\pi} x^2(x, y) \right]^{\frac{1}{2}} = c_w \left[ \frac{M(1 - q^{2N(D-3)})}{2(1 - q^{2(D-3)})} \right]^{\frac{1}{2}}.
\]

Thus, the rough surface in the accepted model is described by six parameters: \( c_w \) (or \( \sigma \)), \( q \), \( K \), \( D \), \( N \), \( M \).

In refs. [4-6], the influence of different parameters on the profiles of surfaces was investigated in detail on the basis of the numerical calculations of the Weierstrass function.

3. Light scattering on surface fractal structures

The scheme of experiment on light scattering by the surface \( S \) is shown in Figure 3. Let us consider the wave falling on the rough surface \( S \) at an angle \( \theta_1 \) and scattering at a polar angle \( \theta_2 \) and an azimuthal angle \( \theta_3 \) in the spherical coordinate system. The gloss coefficient for the coating surface is determined as the ratio

\[
g = \frac{g_{S}}{g},
\]

where \( \langle I_s \rangle = \langle \frac{E_S^2}{I_0} \rangle \) and \( I_0 \) are the average intensity of scattering light on the ensemble of surfaces at the angle \( \theta_1 = \pi/8 \) and \( \theta_1 = 0 \) correspondingly. Therefore, to compare with the experimental data it is necessary to calculate the average intensity of scattering light.

We will find the scattered field \( E_S(\vec{r}) \) after its interaction with the fractal surface (1) on the basis of the scalar Kirchhoff method [8]. This method allows to find the scattered field under the following conditions: (1) the incident wave is mono-chromatic and plane; (2) the scattered surface is rough inside a rectangle \((-X < x_0 < X, -Y < y_0 < Y)\) and smooth outside the borders; (3) the size of the rough site is much larger than the length of the incident wave; (4) the reflection coefficient is the same at all points of the surface; (5) the scattering field is observed far enough from the screen surface [3-7].

**Figure 3.** The scheme of experiment on light scattering by the surface \( S \): \( D \) is detector, \( \theta_1 \) is a falling light angle; \( \theta_2 \) is a polar angle; \( \theta_3 \) is an azimuthal angle.

**Figure 4.** The gloss coefficient for the coating surface versus scattering angles \( \theta_2 \) and \( \theta_3 \). The parameters of Eq.(1) \( N = 5, M = 10, D = 2.5, q = 3 \).
Under these conditions, the scattered field is expressed by the following formula:

\[ E_s(\vec{r}) = -ikrF(\theta_1, \theta_2, \theta_3) \frac{e^{ikr}}{2\pi r} \int_{S} \exp(ik\Phi(x_0, y_0)) \, dx_0 \, dy_0 + E_e(\vec{r}), \]  

(5)

where \( k \) is the wave number of the incident wave; the function \( F(\theta_1, \theta_2, \theta_3) = -\frac{R}{i\pi c} (A^2 + B^2 + C^2) \) is an angle factor; \( R \) is the scattering coefficient; \( \Phi(x_0, y_0) = Ax_0 + By_0 + Cz(x_0, y_0) \) is a phase function; \( h(x_0, y_0) = z(x_0, y_0) \); \( A = \sin\theta_1 - \sin\theta_2 \cos\theta_3 \); \( B = -\sin\theta_2 \sin\theta_3 \); \( C = -\cos\theta_1 - \cos\theta_2 \). The expression (5) may be written in the form: \( E_e(\vec{r}) = -\frac{R}{c} \frac{e^{ikr}}{4\pi r} (A_1 + B_1) \), where the coefficients are expressed thru the integrals:

\[ I_1 = \int_{-\infty}^{\infty} \left[ e^{ik\Phi(x_0, y_0)} - e^{ik\Phi(-x_0, y_0)} \right] dy_0, \quad I_2 = \int_{-\infty}^{\infty} \left[ e^{ik\Phi(x_0, y)} - e^{ik\Phi(x_0, -y)} \right] dx_0. \]

(6)

Having taken integrals (6) using the formula \( e^{i\xi \sin\phi} = \sum_{n=-\infty}^{\infty} I_n(z) e^{i\xi n} \), where \( I_n(z) \) is the Bessel function of integer order \( n \), it is possible to obtain the expression:

\[ E_s(\vec{r}) = -2ikFXY \frac{e^{ikr}}{\pi r} \sum_{l(r, s)} \left\{ \left[ \prod_{u} l_{uw} \right]_{l_s} (\xi_u) \exp[i \sum_{nm} l_{nm} \varphi_{nm}] \right\} \times \text{sinc} (kAX) \text{sinc} (kBY) + E_e(\vec{r}) \]

(7)

with the following notations are used: \( \sum_{l(r, s)} \equiv \sum_{s_0=0}^{\infty} \sum_{s_1=0}^{\infty} \ldots \sum_{s_{(N-1)}=0}^{\infty} \sum_{s_{N}=-\infty}^{\infty} \prod_{u} \Pi_{l_w, s_u} \), \( \sum_{nm} = \sum_{n=0}^{N} \sum_{m=0}^{M} \xi_u \equiv k c_n C q^{(D-3)u} \text{sinc} x, k A = k A + K \sum_{nm} q^n l_{nm} \cos \frac{2\pi m}{M} \), \( K \) is the intensity characterizes scattering by particular realization of surface \( z(x, y) \) with the usual phase \( \varphi_{nm} \).

Calculating \( I_s \rightarrow =< E_s \vec{E}_s > \) and using Equation (8), the exact expression can be obtained:

\[ < I_s > = \left[ \frac{F(\theta_1, \theta_2, \theta_3)}{c \cos \theta_1} \right]^2 \sum_{l(r, s)} \left\{ \prod_{u} l_{uw} \right\}_{l_s} (\xi_u) \text{sinc}^2 (kAX) \text{sinc}^2 (kBY) \]  

\[ + \left[ \frac{R(A^2 + B^2)}{2 c \cos \theta_1} \right]^2 \text{sinc}^2 (kAX) \text{sinc}^2 (kBY). \]

(9)

While the expression (9) contains an infinite sum, using it for numerical calculations appears to be inconvenient. An essential simplification can be reached in the case \( \xi_n < 1 \). Using the Bessel function expansion in the series and neglecting members of orders greater than \( \xi_n \), an approximate expression can be obtained for the average intensity:

\[ < I_s > \approx \left[ \frac{F(\theta_1, \theta_2, \theta_3)}{c \cos \theta_1} \right]^2 \left\{ \left( 1 - (kqC)^2 \right) \text{sinc}^2 (kAX) \text{sinc}^2 (kBY) + \frac{1}{2} \sum_{nm} q^{2(D-3)n} \text{sinc}^2 \left( kA + Kq^n \cos \frac{2\pi m}{M} \right) \right\} \sum \text{sinc}^2 \left( kB + Kq^n \cos \frac{2\pi m}{M} \right) \]  

\[ + \left[ \frac{R(A^2 + B^2)}{2 c \cos \theta_1} \right]^2 \text{sinc}^2 (kAX) \text{sinc}^2 (kBY). \]

(10)
4. Numerical results

On the base of expressions (1), (4) and (10) the numerical modeling of geometrical and optical properties of light scattering with polymer coatings is investigated, the diagrams of scattering (indicatrices for different incident angles $\theta_1$) and the gloss coefficient versus polar ($\theta_2$) and horizontal ($\theta_3$) scattering angles for fractal surfaces of textured polymer coatings of rolled metal were calculated. A root-mean-square value $\sigma$, a surface’s fundamental wave number $K$, and dimensions $X, Y$ of the surface fragment are expressed in $k$-units because the wave number $k$ of the incident wave is used in the form of combinations $k\sigma, kX,$ and $kY$. The Frenel reflection coefficient for a surface is taken as $R = 1$.

An analysis of the scattering indicatrices shows the scattering is symmetrical relatively the plane of incidence and it is maximal intensity in the direction $\theta_3 = 0$. The scattering wave is observed in the cone of lateral directions relatively the normal direction $\theta_2 = 0$. When the incident angle increases, the incident wave as though “stops to notice” the height of imperfections, so their contribution diminishes. The registered scattering peculiarities are a consequence of a combination of both the chaotic character and self-similarity of a scattering rough fractal surface.

5. Conclusion

The gloss coefficient for the coating surface vs. scattering angles $\theta_2$ and $\theta_3$ is shown on Figure 4. Thus, this coefficient differs from zero in other lateral directions: over the interval $\theta_2 \in [0, \pi/3]$ (“forward” scattering) and $\theta_2 \in [0, -\pi/3]$ (“back” scattering). Therefore, the gloss detector, setting in the mirror direction $\theta_2 = -\theta_1 = -\pi/8$, measures more less light intensity from the rough surface than from the smooth one. Therefore, it’s necessary to develop a special convergence experimental technique for such metal coatings allowing identifying a correspondence between the gloss, colour and the texture of the sample surfaces.

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