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Letter to the Editor

Influence of fractal surface roughness on reflectance*

M. ŁĄTKA, K. JEZIERSKI

Institute of Physics, Technical University of Wrocław, Wybrzeże Wyspiańskiego 27, 50–370 Wrocław, Poland.

The new approach of studying the influence of surface roughness on the reflectance is presented. The reflectance for the generated fractal surface is calculated in Fresnel-Kirchhoff approximation. The results are discussed taking into account the existing theories.

1. Introduction

The influence of surface roughness on the reflection spectrum has been widely investigated [1]–[4]. This problem is important, e.g., when the reflectance experimental data are used for further calculations. In the Kramers-Kronig analysis the surface roughness can substantially change the values of optical constants being determined [5]. The influence of surface roughness on reflectance can be very useful for the nondestructive characterization of surface irregularities [3], [6]. For this purpose both the model of surface roughness and the method of calculation of the scattered light are required. Many investigations have confirmed that the surfaces of most materials are fractals, that is, irregularities and defects are self-similar upon variations of resolution [7]–[8].

In this paper the fractal idea was used to generate rough surface. Then the reflectance at normal incidence was calculated in the Fresnel-Kirchhoff approximation [9].

2. Surface generation

This simple midpoint displacement method [7] was applied to generate one dimensional rough surface $z(x)$. At the beginning the midpoint of the horizontal line segment is deflected up or down by a random amount. Each of the two resulting line segments is then subdivided and perturbated in the same way. This process is continued for a given number of iterations. In each iteration the coordinates x, z of a generated point are given by:

$$x = (x_1 + x_2)/2,$$
$$z = (z_2 + z_2)/2 + F(D) \quad (1)$$

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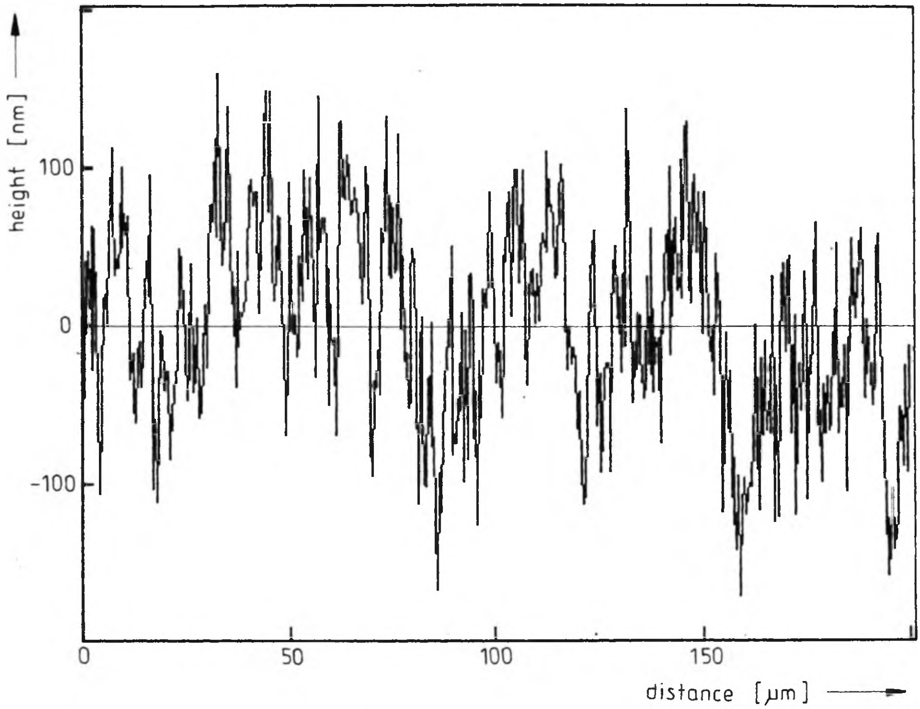

Fig. 1. Profile of the simulated surface

where (x_1, z_1), (x_2, z_2) are a given line's endpoints. The F function is pseudorandom number generator with the Gaussian distribution on interval $[-D, D]$. Each time the iteration is completed the D value is reduced in order to keep the random fluctuations in scale with the size of the segment being varied. The profile of the generated surface obtained after $n = 9$ iterations is plotted in Fig. 1. The further calculations presented in this paper are performed for this surface.

3. Calculations of reflectance

In the calculations of the reflectance at normal incidence both specular and nonspecular reflection was taken into account. The classical Fresnel-Kirchhoff approximation for the diffraction formula as well as the approximation [9] valid for the nearly plane surface were applied. Thus, the electric field $\mathscr{E}$ is given by the following formula:

$$\mathscr{E} = C \iint \exp[-i(\vec{k}_d - \vec{k}_i)\vec{r}]\, dx\, dy \tag{2}$$

where factor C is of little concern in the present discussion; $\vec{k}_i$ and $\vec{k}_d$ are the wave vectors of the incident and diffracted waves, respectively; $\vec{r}$ is the position vector of a given surface element. The integration in (2) is taken over the mean surface level chosen as x, y plane.

Due to the one dimensional character of the generated surface the formula (2) was used in the form

$$\mathscr{E}(\theta) = C_1 \int_{-L}^{L} \exp\{-ik[x\sin\theta + z(1+\cos\theta)]\}\, dx \tag{3}$$

where the configuration of the vectors was following: $\vec{k}_i = (0, 0, -k)$, $\vec{k}_d = (k\sin\theta, 0, k\cos\theta)$, $\vec{r} = (x, y, z)$; $2L$ is the length of the surface. The generated surface is consisted of $N = 2^n$ segments each described as follows:

$$z(x) = z_{0j} + m_j(x - x_{0j}) \tag{4}$$

where m_j is the slope of the j-th segment and (x_{0j}, z_{0j}) – coordinates of the segment's midpoint. In this case, the relations (3) and (4) give

$$\mathscr{E} = C_1 \sum_{j=1}^{N} \exp\{-ik[x_{0j}\sin\theta + z_{0j}(1+\cos\theta)]\} \times 2\tau \,\mathrm{sinc}\{k\tau[\sin\theta + m_j(1+\cos\theta]\} \tag{5}$$

where $\tau = L/N$. For the flat surface, $z(x) = 0$, the equation (3) leads to the following expression:

$$\mathscr{E}_0 = C_1 2L \,\mathrm{sinc}(kL\sin\theta). \tag{6}$$

We are interested in the ratio R/R_0, where R is the reflectance for the rough surface and R_0 is the reflectance for the flat one. When the acceptance angle of the measuring system is θ_0 the value of R/R_0 is given by the formula

$$R/R_0 = \left| \int_{-\theta_0}^{\theta_0} \mathscr{E}(\theta)\, d\theta \Big/ \int_{-\theta_0}^{\theta_0} \mathscr{E}_0(\theta)\, d\theta \right|^2. \tag{7}$$

The ratio R/R_0 can be calculated as the function of wave vector $\vec{k}$ as well as the function of photon energy $E = c\hbar k$.

4. Results and discussion

The calculations of $R/R_0(E)$ have been performed for the acceptance angle $\theta_0 = 3°$ and the results have been plotted in Fig. 2. In order to compare these results with those obtained from the Porteus [1] and Beckmann [2] theories the values of r.m.s. roughness σ and the correlation length T are required. The value of $\sigma = 66$ nm was obtained from the fitting the Gaussian function to the height distribution of the surface (see Fig. 3). The slope distribution for this surface is presented in Fig. 4. The correlation length $T = 1550$ nm was derived from the initial portion of the autocovariance function [10], see Fig. 5.

According to the Porteus theory [1] R/R_0 is given by

$$R/R_0 = \exp(-4k^2\sigma^2) + [1 - \exp(-4k^2\sigma^2)]\,[1 - \exp(-k^2\theta_2^2 T^2/4)]. \tag{8}$$

For this formula with the increase of energy the value of R/R_0 tends to 1. This

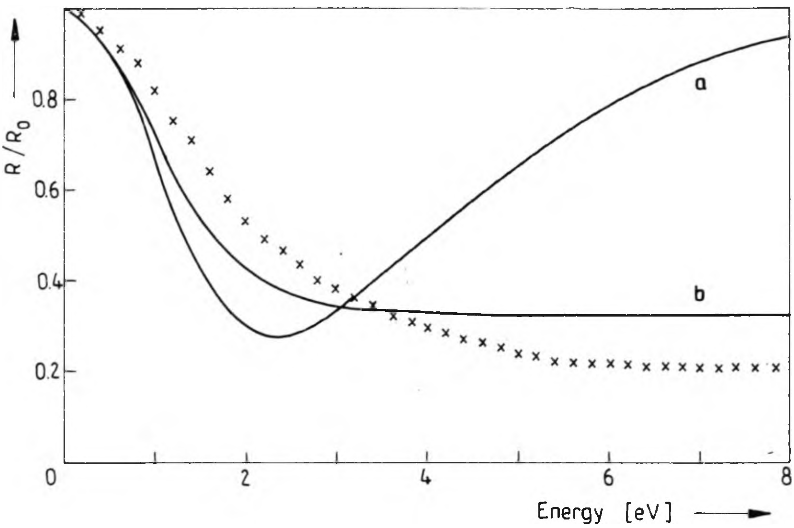

Fig. 2. Influence of the surface roughness on reflectance according to the calculations for the simulated surface (crosses), according to Porteus theory (curve a) and to Beckmann theory (curve b). The curves a and b were determined for the same parameters $\sigma = 66$ nm, $T = 1550$ nm

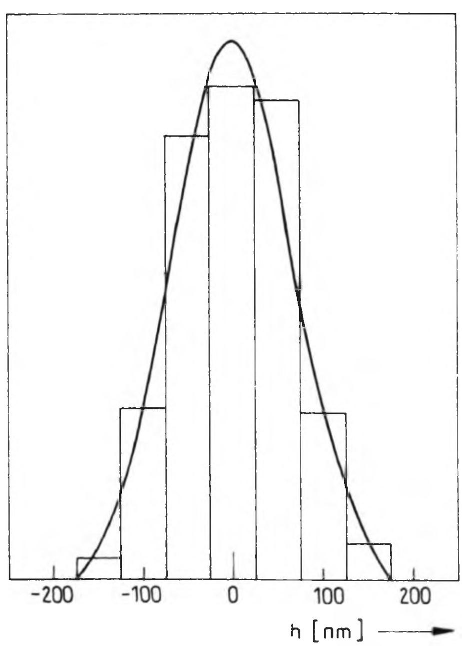

Fig. 3. Histogram of height distribution for the simulated surface and the best Gaussian fit with $\sigma = 66$ nm

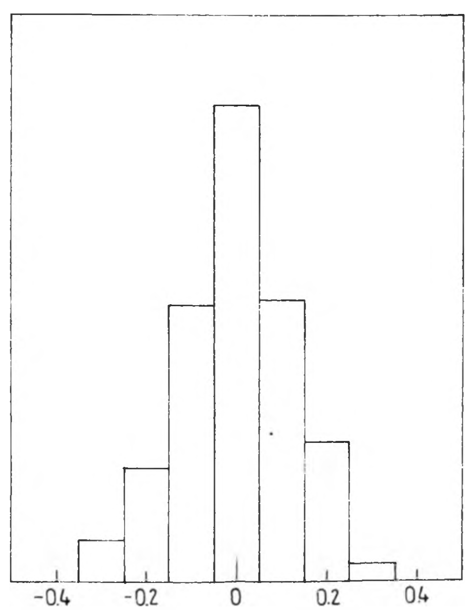

Fig. 4. Histogram of slope distribution for the simulated surface

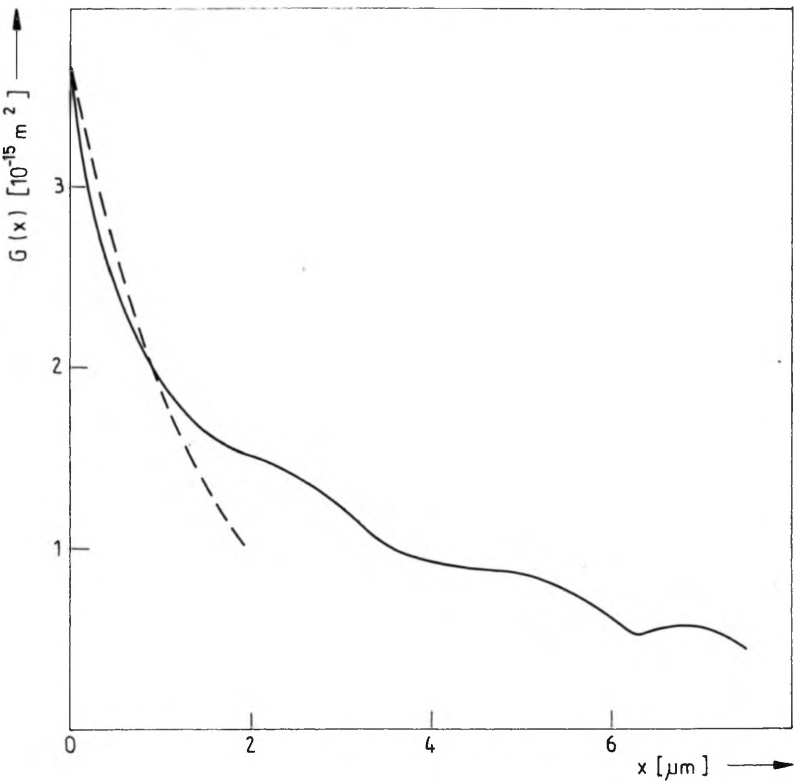

Fig. 5. Initial portion of autocovariance function for the simulated surface (broken line – the best exponential fit with $T = 1550$ nm)

behaviour is the consequence of the chosen model in which the surface is consisted of facets parallel to the mean surface level.

From the Beckmann theory the following relation can be obtained [5]

$$R/R_0 = \exp(-4k^2\sigma^2)\left[1 + \frac{\sqrt{\pi}\,T\,\theta_0}{2\,L\,R_0}\sum_{m=1}^{\infty}\frac{(2k\sigma)^{2m}}{m!\sqrt{m}}\exp(-\theta_0^2 k^2 T^2/4m)\right]. \tag{9}$$

In Figure 2 we can see the qualitative agreement between R/R_0 curves derived from the equation (9) and according to the model of the surface described in this paper. Such behaviour of R/R_0 curve is expected from the experiment.

5. Conclusions

Our preliminary results confirmed that the fractal model for the surface roughness generation is applicable. The $R/R_0(E)$ function has the expectable behaviour in wide energy range. The method presented here produces the surfaces of different height distribution revealing the possibility of reproducing the height distributions encountered in the experiment [11]. Therefore, this method seems to be very promising for characterization of surface roughness from $R/R_0(E)$ experimental data. For this purpose we are developing much more advanced algorithm of surface roughness analysis with the help of the fractal approach.

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Влияние фрактальных неравностей поверхности на коэффициент отражения

Представлен новый подход для исследования влияния неравностей поверхности на коеффициент отражения. В приближении френела–Киргофа рассчитали коэффициент отражения для генерированной фрактальной поверхности. Обсуждены полученные результаты и сравнены с результатами существующих теорий.