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# Light scattering by a rough surface of human skin. 2. Diffuse reflectance

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*Abstract.* **Based on the previously calculated luminance factors, we have investigated the integral characteristics of light reflection from a rough surface of the skin with large-scale inhomogeneities under various conditions of the skin illumination. Shadowing of incident and scattered beams by relief elements is taken into account. Diffuse reflectances by the Gaussian and the quasi-periodic surfaces are compared and, in general, both these roughness models are shown to give similar results. We have studied the effect of the angular structure of radiation multiply scattered deep in the tissue and the refraction of rays as they propagate from the dermis to the surface of the stratum corneum on the reflection characteristics of the skin surface. The importance of these factors is demonstrated. The algorithms constructed can be included in the schemes of calculation of the light fields inside and outside the medium in solving various direct and inverse problems of optics of biological tissues.**

***Keywords:*** *rough surface, skin, diffuse reflectance of light, shadowing, multiple scattering, refraction, biological tissues.*

## 1. Introduction

The study of light propagation through the interface between two media has a very long history. Well-known are the laws of geometrical optics for reflected and refracted rays and the Fresnel formulas for reflection and transmission coefficients by a smooth (flat) interface. However, the surfaces of real objects are characterised in a greater or lesser degree by roughness. Accounting for the effects of the surface structure on the transmission of light is crucial in solving a variety of theoretical and applied problems in the field of spectroscopy, photometry, lighting engineering, radiolocation, geophysics, etc. With regard to biomedical optics, we have derived analytical formulas for the polar and azimuth dependences of the luminance factors of light reflected (and transmitted) by the rough surface of the skin [1]. The basis of these formulas was an asymptotic solution of Maxwell's equations in the geometrical optics approximation for a dielectric surface with large-scale relief elements [2, 3] and the model of the surface roughness of the human skin [4]. For many applications of biomedical optics, of particular interest are the integral characteristics of light reflection and transmission at the skin – surrounding medium interface. These applications include the development and optimisation of the methods of low-level laser therapy, including photodynamic and laser hyperthermia, the development of algorithms of diagnostics of biological tissues under *in vivo* conditions, and the determination of their structural and biophysical parameters by the characteristics of the scattered radiation, and many others. The authors of papers [5 – 7] proposed analytical algorithms for calculating the optical fields inside and outside the biological tissues, based on the adding-doubling method [8], in which the surface of the skin is regarded as a separate layer. Its integrated diffuse reflectance $R$ and transmittance $T$ directly enter into the final formula. Because $T \equiv 1 - R$, we will below consider only diffuse reflectance. In the vast majority of works on optics of biological tissues, the surface of the skin is assumed smooth, so that the coefficients of its reflectance in the case of directional ($R$) and completely diffuse ($R^*$) illumination can be easily estimated by the Fresnel formulas. Thus, if we assume that the refractive index $n$ of the surface of the stratum corneum of the skin varies from 1.33 (water) to 1.55 [9, 10], we obtain the ranges of variation in diffuse reflectance $R_1^*$ and $R_2^*$ from 0.066 to 0.099 and 0.465 to 0.624, respectively (subscript 1 refers to illumination of from outside the medium and subscript 2 – from the biological tissue). When processing large arrays of experimentally obtained diffuse reflectance spectra of the skin tissue, $R_\infty(\lambda)$ [11, 12], the coefficient $R_2^*$ was used as a fitting parameter. It was found that for the results of calculations [6] and measurements of $R_\infty(\lambda)$ to be consistent, the $R_2^*$ values must be in the range from 0.2 to 0.4, and the calculation algorithm [6] should include the dependence of $R_2^*$ on the wavelength $\lambda$. This range is clearly different from that given above (0.465 – 0.624) due to changes in the refractive index. This was the main motivation for the study of diffuse reflectance by a rough surface of the skin in this paper.

A number of publications are devoted to the numerical solution of the radiative transfer equations in a biological tissue using Monte Carlo simulation with the skin surface roughness taken into account [13 – 16]. The diffuse reflectance is not directly included in these equations, since the passage of light through the medium boundary is analysed by simulating the trajectories of the photons. However, the data on the reflection and transmission coefficients can be used for indirect verification of the algorithms of the corresponding numerical schemes. Note that Lu et al. [13] considered the

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surface with a Gaussian probability density of surface elevations and a Gaussian correlation function, and the authors of papers [13–16] – a randomly inhomogeneous quasi-periodic (sinusoidal) surface with elevations $\zeta(r) = \zeta_m \sin(\omega r + \theta)$ above the plane $z = 0$ and with the phase $\theta$ uniformly distributed on the interval $[0, 2\pi]$ ($r$ is the length of the radius vector in the plane $xy$, see Fig. 1 in [1]).

The aim of this work is to study spectral diffuse reflectance of light by a rough surface of the skin for Gaussian [13, 17] and quasi-periodic [14–16] models taking into account the mutual shadowing of the relief elements and to assess the limits of changes in these coefficients at typical structural and biophysical parameters of the tissue. The basis of the research involves the models of the optical and structural properties of the medium [9, 10, 18–21], including the parameters of the interface roughness [4, 13–16], analytical methods for solving the radiative transfer equation [6, 7, 22] in biological tissues and results of calculation of the luminance factor of the skin surface [1–3].

## 2. Calculation formulas for diffuse reflectance of Gaussian and quasi-periodic surfaces

For a surface with a known luminance factor $\rho(\chi,\varphi,\psi)$ of the reflected light, which depends on the polar ($\chi$) and azimuth ($\varphi$) observation angles and the polar angle $\psi$ of incidence (the azimuth of the incident beam is assumed zero), the diffuse reflectances of light, $R$ and $R^*$, are respectively defined [22, 23] as

$$R(\psi) = \frac{1}{\pi}\int_0^{2\pi} \mathrm{d}\varphi \int_0^{\pi/2} \rho(\chi,\varphi,\psi)\sin\chi\cos\chi \mathrm{d}\chi, \tag{1}$$

$$R^* = 2\int_0^{\pi/2} R(\psi)\sin\psi\cos\psi \mathrm{d}\psi. \tag{2}$$

In paper [1], using the results of [2, 3], we obtained an analytical expression for $\rho(\chi,\varphi,\psi)$:

$$\rho(\chi,\varphi,\psi) = \frac{\pi I(\chi,\varphi,\psi)\, Q(a,b)}{E_0 S_0 \cos\chi}, \tag{3}$$

where the luminous intensity of light from an illuminated macro surface ($z = 0$) of area $S_0$ is

$$I(\chi,\varphi,\psi) = \frac{E_0 S_0}{4\cos\psi} r_F(\eta) \frac{q^4}{q_z^4} W\left(\gamma = -\frac{\boldsymbol{q}_\perp}{q_z}\right); \tag{4}$$

$E_0$ is the macro surface illumination at an angle $\psi$ of incidence of rays; $r_F(\eta)$ is the Fresnel reflection coefficient that depends on the local angle $\eta$ of incidence of light on micro areas; $q = |\boldsymbol{q}| = |\boldsymbol{\kappa} - \boldsymbol{\kappa}_0|$; $\boldsymbol{\kappa}$ and $\boldsymbol{\kappa}_0$ are the unit vectors along the propagation direction of incident and reflected waves, respectively; and $q_z$ and $\boldsymbol{q}_\perp$ are the projections of the vector $\boldsymbol{q}$ on the $z$ axis and the plane $xy$ (see Fig. 1 in [1]). The probability density $W(\gamma)$ of random slopes for the Gaussian and sinusoidal surfaces relative to the plane $z = 0$ have, respectively, the form [3, 4]:

$$W(\gamma) = \frac{1}{2\pi D_\gamma} \exp\left(-\frac{\gamma^2}{2D_\gamma}\right), \tag{5}$$

$$W_s(\gamma) = \begin{cases} \dfrac{1}{\pi\sqrt{\gamma_m^2 - \gamma^2}} & \text{at } |\gamma| \leqslant \gamma_m, \\ 0 & \text{at } |\gamma| > \gamma_m, \end{cases} \tag{6}$$

where $\gamma_m = \omega\zeta_m$ is the maximum slope of a sinusoid to the plane $xy$; and $\omega$ and $\zeta_m$ are its frequency and amplitude. The function $Q(a, b)$ takes into account the mutual shadowing of relief elements [1, 3]: $Q(a, b) = [1 + \Lambda(a) + \Lambda(b)]^{-1}$, where for the Gaussian and sinusoidal surfaces we have [3]

$$\Lambda(a) = \frac{1}{2a}[\sqrt{2/\pi}\exp(-0.5a^2) - a\,\mathrm{erfc}(a/\sqrt{2})], \tag{7}$$

$$\Lambda_s(a) = (1/\pi)[\sqrt{(2/a^2) - 1} - \arccos(a/\sqrt{2})] \text{ at } a \leqslant \sqrt{2}; \tag{8}$$

$a = \cot\psi/\langle\gamma_{(s)}\rangle$; $b = \cot\chi/\langle\gamma_{(s)}\rangle$; $\langle\gamma_{(s)}\rangle = [D_{\gamma(s)}]^{0.5}$; and $D_{\gamma(s)}$ is the variance of the Gaussian (sinusoidal) surface slopes. When $a > \sqrt{2}$, instead of (8) we have $\Lambda_s(a) \equiv 0$. Since $D_{\gamma(s)} = (\gamma_m)^2/2$ [4], the maximum value is $a = \sqrt{2}$. This means that rays incident or scattered at small angles $\psi$ or $\chi$, respectively (large values of $\cot\psi$ or $\cot\chi$), are not shadowed by the relief elements due to a limited inclination of the quasi-periodic surface. In this connection, the above identity holds true. We note here that for the Gaussian surface the slope $\gamma$ can be any value because the probability density (5) is positive over the entire range $0 \leqslant \gamma < \infty$. It follows from (7) and (8) that, at large $a$ and $b$, i.e., at small values of $\psi$, $\chi$ and (or) $D_{\gamma(s)}$, the shadowing effect is not observed, since $\Lambda(a)$, $\Lambda(b) \to 0$.

As seen from (6), the probability density $W_s(\gamma) \to \infty$ when $\gamma = \gamma_m$. The reasons of this are discussed in [3]. Despite this feature, the function $W_s(\gamma)$ is integrable, but this is inconvenient in numerical calculations of double and triple integral (1) and (2) over the angles $\chi$, $\varphi$ and $\psi$. For the calculations it is easier to consider reflection of light by a quasi-periodic surface from the point of view of the angular distribution function $f(\beta)$ of micro areas [1, 4, 23], whereas the integration in (1) and (2) should be performed by the allowed values of the polar ($\beta' = \pi - \beta$, $\psi$) and azimuth ($\varepsilon$, $\phi$) angles specifying, respectively, the position of the local outward normal to micro areas and luminous intensity of incident light in the new coordinate system $x'y'z'$ (see Fig. A1 in the Appendix). We obtained [4] for the function $f(\beta)$ of a sinusoidal surface the expression:

$$f(\beta) = \frac{4\arccos[(\tan\beta)/\gamma_m]}{\pi^3 \sin\beta\cos^3\beta\sqrt{\gamma_m^2 - \tan^2\beta}} \text{ at } \tan\beta \leqslant \gamma_m. \tag{9}$$

When $\tan\beta > \gamma_m$, the function $f(\beta) = 0$ because $\gamma_m$ is the maximum slope of the surface. When $\tan\beta \to \gamma_m$, the function $f(\beta) \to (4/\pi^3)[\gamma_m^2/(1 + \gamma_m^2)]$, i.e., in contrast to $W_s(\gamma)$, takes a finite value. For this reason it is easier to use the function $f(\beta)$ in calculations of the diffuse reflectance.

Then, as shown in the Appendix, the diffuse reflectance of a rough surface illuminated along the normal to the plane $x'y'z'$ (Fig. A1) has the form

$$R(\psi = 0) = 2\pi\int_0^{\pi/4} f(\beta)\sin\beta\cos\beta\, r_F(\beta)\,\mathrm{d}\beta. \tag{10}$$

Note that the integral in (10) is taken up to $\pi/4$, because stronger inclined areas do not contribute to the diffuse reflectance, and reflect light only in the forward hemisphere relative to the illumination direction. When a completely diffuse flux is incident on the surface,

$$R^* = 4\Big\{\int_{\pi/2}^{3\pi/4} f(\pi-\beta')\sin\beta' \mathrm{d}\beta' \Big[\int_{3\pi/2-2\beta'}^{\pi/2}\sin\psi \mathrm{d}\psi \int_{\varkappa}^{\pi}\cos\eta\, r_{\mathrm{F}}(\eta)\,\mathrm{d}\phi$$

$$+ \int_0^{3\pi/2}\sin\psi \mathrm{d}\psi\int_{\pi/2}^{\pi}\cos\eta\, r_{\mathrm{F}}(\eta)\,\mathrm{d}\phi\Big] + \int_{3\pi/4}^{\pi} f(\pi-\beta)\sin\beta' \mathrm{d}\beta$$

$$\times\Big[\int_0^{\pi/2}\sin\psi \mathrm{d}\psi\int_{\pi/2}^{\pi}\cos\eta\, r_{\mathrm{F}}(\eta)\,\mathrm{d}\phi + \int_0^{2\beta'-3\pi/2}\sin\psi \mathrm{d}\psi$$

$$\times\int_0^{\pi/2}\cos\eta\, r_{\mathrm{F}}(\eta)\,\mathrm{d}\phi + \int_{2\beta'-3\pi/2}^{\pi/2}\sin\psi \mathrm{d}\psi\int_{\varkappa}^{\pi/2}\cos\eta\, r_{\mathrm{F}}(\eta)\,\mathrm{d}\phi\Big]\Big\}, \quad (11)$$

where $\varkappa = \arccos[-1/(\tan\psi \tan 2\beta')]$, and angle $\eta$ of incidence is given by formula (A3).

## 3. Results and discussion

### 3.1. Diffuse reflectance with mutual shadowing of surface relief elements taken into account

It is interesting to find out when shadowing effects occur and how significant they are and when they can be neglected. Consider a Gaussian surface. We characterise its roughness by the value of $D_\gamma$, i.e., the variance of the inclination angles of micro areas. Figure 1 shows the dependence of diffuse reflectances $R_{1,2}$ and $R^*_{1,2}$ on $D_\gamma$ in the case of directed and completely diffuse illumination of the skin from outside and inside the tissue. The refractive index of the stratum corneum is $n = 1.55$. The analysis [4] of the experimental data on the human skin roughness degree and of the $D_\gamma$ values used in the theoretical consideration of light propagation through the skin showed that the typical range of the variance is 0.001 – 0.1. This range depends on many factors, such as a person's age, place of skin tests, skin pathology and external effects, including the effects of the environment. In addition, the published data on $D_\gamma$ are insufficient. Therefore, Fig. 1 shows the dependence of the reflection coefficients for a wide range of the variance values as compared with those mentioned above, including a smooth surface ($D_\gamma = 0$). Naturally, the diffuse reflectance in the case of illumination from inside a medium is greater than in the case of radiation incident outside a tissue. At small angles of incidence, the reflection coefficient is less [curves (*1*) and (*2*)] than in the case of diffuse illumination [curve (*4*)]. At large $\psi$ [curve (*3*)], the situation is reversed. This is associated with an increase in the Fresnel reflection coefficient with increasing angle of light incidence.

We showed in [1] that the shadowing effect influences the luminance factors $\rho(\chi,\varphi,\psi)$ at $\chi$ and $\psi$ on the order of 70° or higher. By definition, diffuse reflection is affected in the case of directional illumination of the surface [formula (1)] by the rays with $0 \leqslant \chi \leqslant 90°$, and in the case of diffuse illumination (2) by the rays with $0 \leqslant \psi \leqslant 90°$ as well. Therefore, mutual shadowing of the relief elements is already apparent when the surface is illuminated along the normal, starting with small values of $D_\gamma$. Naturally, with increasing incidence angle $\psi$, especially in the case of diffuse reflection, this effect becomes more significant. Below all the results will be presented with shadowing taken into account.

Worthy of attention is also a marked increase in diffuse reflectance (by about 2 – 4 times) with an increase in the variance when the skin is illuminated along the normal from inside the tissue [curve (*1*) in Fig. 1b]. A similar growth, though to a lesser extent, occurs when the surface is illuminated from outside the medium at small angles of $\psi$ [curves (*1*) and (*2*) in Fig. 1a]. With increasing $D_\gamma$ diffuse reflectance is influenced by two factors. First, the Fresnel reflectance $r_{\mathrm{F}}(\eta)$ from inclined micro areas increases because of the larger local incidence angle $\eta$. Second, the area of the micro areas increases. Both these factors have an impact in 'one direction', leading to the corresponding dependences of diffuse reflectance on $D_\gamma$. With increasing the angle $\psi$, the reflection coefficients as a function of the variance decrease. In this case, the values of $\eta$ can either increase or decrease (see Fig. A1), depending on which side, relative to the local normal to the micro area, the light is incident. The corresponding changes in $r_{\mathrm{F}}(\eta)$ compensate for an increase in the area of the inclined micro areas, which leads to the dependence of the diffuse reflectance (shown in Fig. 1) with increasing surface roughness. Note that at small $D_\gamma$ the skin surface from the point of view of diffuse reflectance behaves as smooth. In general, the range of variation in the reflection coefficients depends stronger on the illumination conditions, than on the degree of skin roughness.

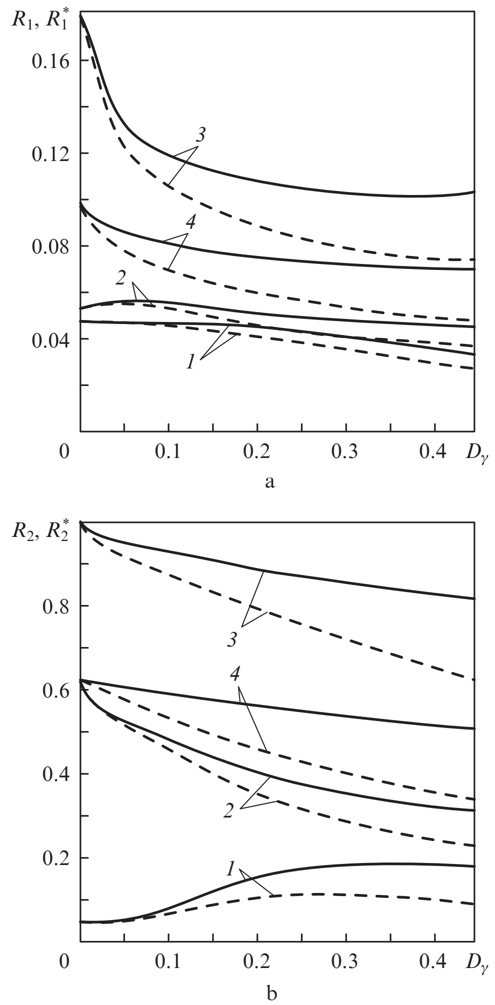


**Figure 1.** Dependences of diffuse reflectance of the rough skin surface on the variance $D_\gamma$ with (dashed curves) and without (solid curves) shadowing effects taken into account for the Gaussian surface under illumination from (a) outside and (b) inside the medium; $\psi$ = (*1*) 0, (*2*) 20°, (*3*) 70°, diffuse illumination (4).

### 3.2. Comparison of diffuse reflectance for Gaussian and quasi-periodic surface models

It was noted above that to describe the degree of the skin roughness, use was made of Gaussian (5) [13, 17] and quasi-periodic (6) [14–16] models. In formulas (3) and (4) for the luminance factor, the structure of the surface is treated only as a probability density of its slopes. The remaining factors in (3) and (4) are angular functions that do not depend on the relief parameters. Naturally, the difference between the luminance factors of the reflected light is the same as that between the dependences $W(\gamma)$ and $W_s(\gamma)$. It is expected that the reflection coefficients $R_{1,2}$ and $R^*_{1,2}$ for the two models will be closer to each other because the details of the angular dependences of $W(\gamma)$ and $W_s(\gamma)$ are averaged during integration. To compare the values of diffuse reflectance in these two cases, we choose the probability densities at which $D_\gamma = D_{\gamma s}$. The results of comparison are listed in Table 1. At first, we note the general properties that do not depend on the type of surface. Obviously, the diffuse reflectance in the case of diffuse illumination is much larger than in the case of directed illumination, which is due to an increase in the Fresnel coefficient for oblique rays. In the case of small variances, at approximately $D_\gamma < 0.05$ for normal and at $D_\gamma < 0.01$ for diffuse illumination, the diffuse reflectance of a roughened surface is the same as for a smooth one. With increasing $D_\gamma$, differences between reflection coefficients begin to manifest as compared with the case of $D_\gamma = 0$. Here, two factors come into force, which affect the diffuse reflectance in opposite directions. First, the fraction of inclined rough surface micro areas increases, which in the case of illumination along the normal leads to an increase in the average local angle $\eta$ of incidence of the light, larger Fresnel reflection coefficient and, consequently, to an increase in diffuse reflection. It is clear that during diffuse illumination, this factor is not so significant. Second, with increasing $D_\gamma$ shadowing effects that reduce the diffuse reflectance are enhanced. Mutual shielding of the relief elements affects diffuse reflectance stronger than the increase in the angle $\eta$ of incidence. Only at large values of $D_\gamma$ and under directional illumination of the medium from inside, we observe a marked maximum of the diffuse reflectance both for the Gaussian and the sinusoidal surface, which is associated with a local angle of incidence. In this case, the Fresnel reflection coefficient dramatically increases with increasing $\eta$ and becomes equal to unity even at its relatively small values (approximately 40° or greater at $n = 1.55$), which correspond to total internal reflection. When the medium is illuminated from outside, this increase in $r_F(\eta)$ is not observed.

As can be seen from Table 1, the diffuse reflectances for the two types of the skin surface are close to each other in a wide range of $D_\gamma$ values. In the case of diffuse illumination of the medium from both outside and inside, the relative differences between them do not exceed 5%–7%. When illuminated along the normal, the differences are more significant, being approximately twice large in the vicinity of the mentioned maximum of diffuse reflectance as a function of the variance $D_\gamma$. The reason for this is as follows. It is obvious that the angular dependences of $W(\gamma)$ and $W_s(\gamma)$ are generally different. When $D_{\gamma s} < 0.45$, the maximum value of $\gamma_m$ is $(2D_{\gamma s})^{1/2} \approx 0.95$ for a quasi-periodic surface and the corresponding angle of inclination of micro areas is about 54°. At such angles and normal incidence of light, shadowing does not affect the luminance factor [1]. On the other hand, small values of $\gamma_m$ cause small local angles $\eta$ of incidence. For a Gaussian surface, there are no restrictions on $\gamma_m$, and so of importance here is shadowing and growth of the Fresnel reflection coefficient. As explained above, the impact of these factors on the diffuse reflectance is different. Therefore, for the Gaussian surface at $D_\gamma \approx 0.2$ and for the sinusoidal surface at $D_{\gamma s} \approx 0.4$, dominant contribution to the increase in diffuse reflectance under incidence of light along the normal to the boundary from outside the medium is associated with an increase in $\eta$. As $D_\gamma$ further increases, shadowing of the reflected rays by the relief elements of the Gaussian surface becomes significant and its diffuse reflectance decreases. In the case of diffuse illumination from the in-depth of the tissue, a decrease in the diffuse reflectance with increasing $D_\gamma$ is due to the screening of the incident light for the two types of the interface and due to the screening of the reflected light for the Gaussian surface.

### 3.3. Diffuse reflectance upon illumination of the skin surface by multiply scattered radiation

Above, we have considered two limiting cases of illumination, i.e., directional and completely diffuse illumination, which made it possible to identify the common features of the behaviour of diffuse reflectance at different values of $D_\gamma$ for the two models of the rough surface. We now analyse the real situation which occurs when radiation is incident from outside the medium along the normal and when the surface of the skin is irradiated from inside by the light scattered back in the tissue in-depth. In this case, the luminance factor $\rho_2(\psi)$ of scattered radiation, which determines the angular structure of skin surface illumination, differs from these extreme cases, which, of course, affects the diffuse reflectance $R'_2$ (the prime refers to an arbitrary exposure of the interface). Note that due to obvious symmetry of the problem, $\rho_2$ is independent of the azimuth angle. Then we can consider only the Gaussian surface because of proximity of its integral characteristics of reflec-

**Table 1.** Diffuse reflectances (%) of the Gaussian and sinusoidal surfaces under normal incidence and completely diffuse incidence of light.

| $D_\gamma$ | Directional radiation | | | | Diffuse radiation | | | |
|---|---|---|---|---|---|---|---|---|
| | Outside | | Inside | | Outside | | Inside | |
| | Gaussian surface | Sinusoidal surface | Gaussian surface | Sinusoidal surface | Gaussian surface | Sinusoidal surface | Gaussian surface | Sinusoidal surface |
| 0 | 4.65 | 4.65 | 4.65 | 4.65 | 9.91 | 9.91 | 62.4 | 62.4 |
| 0.002 | 4.65 | 4.65 | 4.65 | 4.66 | 9.69 | 9.77 | 62.3 | 62.2 |
| 0.013 | 4.65 | 4.65 | 4.67 | 4.68 | 9.0 | 9.25 | 61.3 | 61.5 |
| 0.05 | 4.68 | 4.66 | 5.06 | 4.8 | 7.79 | 8.19 | 57.8 | 58.8 |
| 0.2 | 4.12 | 4.69 | 10.5 | 5.58 | 6.02 | 6.39 | 46.0 | 49.4 |
| 0.44 | 2.67 | 4.83 | 8.86 | 15.6 | 4.78 | 5.08 | 33.7 | 38.0 |

tion and diffuse reflectance of the quasi-periodic surface under diffuse illumination (see Table 1). In this case, the formula for calculating diffuse reflectance takes the form

$$R_2' = \int_0^{\pi/2} R(\psi)\rho_2(\psi)\sin\psi\cos\psi d\psi / \int_0^{\pi/2} \rho_2(\psi)\sin\psi\cos\psi d\psi. \quad (12)$$

According to the asymptotic theory of radiative transfer in a scattering medium [22, 24], the luminance factor $\rho_{ed}(\psi)$ of light passing through the tissue depth to the skin surface is given by [25]

$$\rho_{ed}(\psi) = \Gamma(0)\Gamma(\psi)\{\rho_0(\psi) - \{1 - \exp[-4g(\psi)g_0(0)\sqrt{\mu_{ad}/(3\mu'_{ed})}\,]\}\}. \quad (13)$$

Here $\rho_0(\psi) = 0.5(1 + 4\cos\psi)/(1 + \cos\psi)$ is the luminance factor of an nonabsorbing semi-infinite medium [22]; $g(\psi) = 3(1 + 2\cos\psi)/7$; $\mu'_{ed} = \mu_{ad} + \mu_{sd}(1 - \omega_d)$ is the effective extinction coefficient of the dermis; $\mu_{ad}$ and $\mu_{sd}$ are the absorption and scattering coefficients, respectively; $\omega_d$ is the the average cosine of the scattering indicatrix of the elementary volume of the dermis; and $\Gamma(\psi)$ is the light transmittance by the epidermis illuminated at an angle $\psi$ with respect to the surface normal. In (13) the transmittance of the stratum corneum is not considered, since, due to the smallness of the optical thickness of the layer, it is close to unity. For deriving $\Gamma(\psi)$ [26], we use small-angle approximation of the radiative transfer theory [22]: $\Gamma(\psi) = \exp[-d_e(\mu_{ee} - \mu_{se}F_e)/\cos\psi]$, where $d_e$ is the geometrical thickness of the epidermis; $F_e = 1 - (1 - \omega_e)/3$ is the fraction of light scattered in the epidermis in the 'forward' direction; $\mu_{ee}$ and $\mu_{se}$ are the extinction and scattering coefficients, respectively; and $\omega_e$ is the average cosine of the phase function of the epidermis.

Note that the above parameters of the elementary volume are dependent on the wavelength of incident light, in particular $\omega_d = \omega_e = 0.62 + 0.00029\lambda$ [20] ($\lambda$ is in nm). For an analytical description of other parameters and their relationship with the structural and biophysical characteristics of tissue, use is made of the model of optical properties of the skin [6, 21, 27], constructed on the basis of the published data [9, 10, 18–21]. These parameters are obtained by additive summation of the respective characteristics of the main skin chromophores – tissue, melanin and blood (oxy- and deoxyhaemoglobin). As a result, the model [6, 21, 27] allows one to analytically relate in the range of wavelengths $\lambda = 300$–$1000$ nm the optical properties of each layer of the tissue with the biophysical characteristics – the volume concentration of melanin ($f_m$) and blood capillaries ($C_v$), the degree of blood oxygenation $S$, capillary hematocrit $H$ and the volume fraction $f$ of haemoglobin in red blood cells. By its physical meaning, $f_m$, $C_v$, $H$ and $f$ are the volumes of melanin, capillaries, erythrocytes and haemoglobin per unit volume of the epidermis, dermis, blood and erythrocytes, respectively; and $S$ is the ratio of the oxyhaemoglobin to the total amount of haemoglobin in the blood. The following calculations were performed at fixed $C_v = 0.04$, $S = 0.75$, $H = 0.4$ and $f = 0.25$. The parameter $f_m$ was varied from 0.04 to 0.16, typical for a normal light skin [18, 27]. These characteristics are necessary to determine the spectral luminance factors $\rho_{ed}(\psi)$, specifying the angular structure of illumination of the inner surface of the stratum corneum from inside the medium at different wavelengths. In the model [6, 21, 27], it is also assumed that there is a gradual change in the refractive index between the skin layers, such that light is reflected only from the interface between a rough surface and the surrounding air.

For a biological tissue, there is another mechanism that affects the diffuse reflectance of the skin, $R'_2$. As is known [9, 10], the refractive index $n_i$ of the interstitial fluid is less than the value of $n = 1.55$, typical of the stratum corneum. For example, Bashkatov et al. [10] proposed spectrum approximation $n_i(\lambda)$, giving an interval of its change of about 1.33–1.36 in the wavelength range 300–1000 nm. For simplicity we assume $n_i = 1.33$, independently of $\lambda$. Due to the difference between the values of $n_i$ and $n$, the light beam incident at the angle $\psi$ onto the inner surface of the stratum corneum from the tissue side will experience refraction. In this case, the angular dependence $\rho_{ed}(\psi)$ changes; radiation is concentrated in a narrower range of angles, close to the normal to the skin surface, and its intensity increases. Mathematically, the effect of refraction on the luminance factor $\rho_2(\psi)$ is written in the form:

$$\rho_2(\psi) = \rho_{ed}[\arcsin(n\sin\psi/n_i)](n/n_i)^2. \quad (14)$$

As can be seen from (14), the maximum angle of incidence of light on the interface between from inside the medium is $\arcsin(n_i/n) \approx 60°$ and $\rho_2(\psi) \equiv 0$ for $\psi$ exceeding this angle.

Consider the spectra of diffuse reflectance $R'_2$, obtained by taking refraction into account. The corresponding data are shown in Fig. 2, which presents the dependences of $R'_2(\lambda)$ for a smooth [$D_\gamma = 0$, curves (*1*) and (*2*)] and a rough [$D_\gamma = 0.44$, curves (*3*) and (*4*)] surface, calculated without and with refraction taken into account at different concentrations of melanin $f_m$. The diffuse reflectance spectra exhibit local minima corresponding to the absorption maxima of blood at wavelengths of about 420, 550 and 575 nm. The reason is that with increasing absorption coefficient of the dermis containing blood, the angular pattern of the luminance factor $\rho_{ed}(\psi)$ of backscattered light becomes narrower in $\psi$, so that the local angle of incidence of radiation on the micro areas of the skin surface is generally reduced. Accordingly, this leads to a decrease in the Fresnel reflection coefficient and thus in the value of $R'_2$. With increasing concentration $f_m$, these minima become less noticeable, especially for the rough surface. This is due to the strong attenuation of oblique rays by the epider-

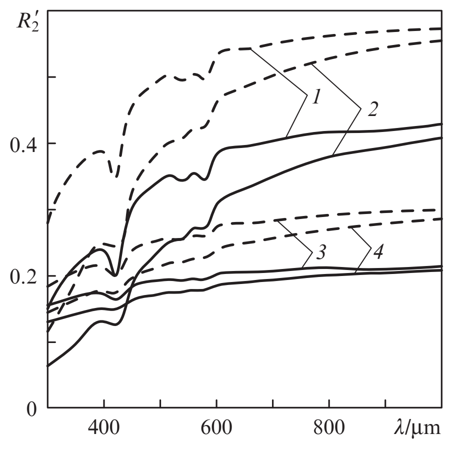


**Figure 2.** Dependence of diffuse reflection $R'_2$ on $\lambda$ without refraction (dashed curves) and with refraction (solid curves) taken into account at $D_\gamma =$ (*1*, *2*) 0 and (*3*, *4*) 0.44, $f_m =$ (*1*, *3*) 0.04 and (*2*, *4*) 0.16.

mis [the presence of $\cos\psi$ in transmittance $\Gamma(\psi)$], so that the concentration of backscattered light in a narrow range of the angles $\psi$ for the stronger absorbing dermis is largely levelled by the influence of the epidermis.

Let us compare the dashed and solid curves (*1*) in Fig. 2, illustrating the effect of the differences in the refractive indices $n$ and $n_i$ on diffuse reflectance for the smooth surface at $f_m = 0.04$, i.e., in the 'pure' form, not 'shaded' by the roughness of the interface. One can see that in the range of $\lambda$ under study, refraction reduces reflectance, which is due to the previously observed narrowing of the angular illumination pattern $\rho_2(\psi)$ as compared with the luminance factor $\rho_{ed}(\psi)$. Somewhat unexpected is the reduction of the spectral values of diffuse reflectance by an approximately constant value 0.13–0.15, which is almost independent of the wavelength. It would seem that in the blue-violet region of the spectrum where the oblique rays are greatly attenuated due to the high absorption by melanin, refraction should influence diffuse reflection weaker than in the red region. To explain this fact, we should analyse the dependences $\rho_2(\psi)$ and $\rho_{ed}(\psi)$. Analysis shows that for the above-mentioned biophysical and structural characteristics of the tissue the equality $\rho_2(\psi) = \rho_{ed}(\psi)$ is fulfilled in the short-wavelength region of the spectrum at the angle $\psi^* \approx 40°$, corresponding to the critical angle of total internal reflection of light from the skin surface. If $\psi > 40°$, the luminance factor is $\rho_2(\psi) > \rho_{ed}(\psi)$, and if $\psi < 40°$, the opposite inequality holds true. The boundary value of the angle $\psi^*$ increases with increasing $\lambda$. Thus, if refraction is not taken into account, a significant fraction of the luminous flux incident on the skin surface with the angular pattern $\rho_{ed}(\psi)$ experiences total internal reflection with the Fresnel reflection coefficient equal to unity. Refraction causes a significant decrease in the fraction of the luminous flux illuminating the interface at angles for which total internal reflection is observed. Thus, the values of $r_F$ and diffuse reflectance decrease. In the red region of the spectrum, refraction noticeably reduces the width of the angular patterns $\rho_{ed}(\psi)$ as compared to the blue-violet region, but a significant fraction of the incident flux experiences total internal reflection. The calculations illustrated by curves (*1*) in Fig. 2 show that when $f_m = 0.04$ the competition between the two considered factors approximately compensates for the corresponding changes in diffuse reflectance, such that its absolute decrease is approximately constant at $\lambda = 300–1000$ nm. With increasing concentration of melanin [curves (*2*), $f_m = 0.16$], more significant is the narrowing of the angular pattern $\rho_2(\psi)$ as compared with total internal reflection, such that the decrease in diffuse reflectance in absolute units due to refraction is greater in the red region than in the blue-violet region (approximately 0.15 vs. 0.05). For the rough surface of the skin with $f_m = 0.04–0.16$, an absolute decrease in the diffuse reflectance with refraction taken into account is always more significant in the red region of the spectrum. With increasing wavelength the effect of the concentration of melanin is waning due to a decrease in its absorption coefficient.

Consider the dependence of $R'_2$ for the angular illumination pattern (13) and (14) on the slope variance $D_\gamma$ of the rough surface of the skin (Fig. 3). First, we note an increase in diffuse reflectance with increasing wavelength for any values of $D_\gamma$. It also follows from Fig. 2 and is caused by the respective broadening of the angular pattern $\rho_2(\psi)$ of the interface illumination. Noteworthy is a clear maximum of the diffuse reflectance in the short-wavelength region at $D_\gamma \approx 0.07–0.08$, when $R'_2$ of the rough surface increases by about 1.3–1.5 times in comparison with the smooth interface. It is due to the increase in the average local angle of incidence of the light on micro areas and in the fraction of inclined relief elements with increasing $D_\gamma$ to specified values. With a further increase in variance, the shadowing effect becomes more pronounced, and diffuse reflectance decreases. When illuminating in the red region of the spectrum a similar maximum of $R'_2$ is expressed much weaker and occurs at low values of $D_\gamma$, typical of a virtually smooth surface.

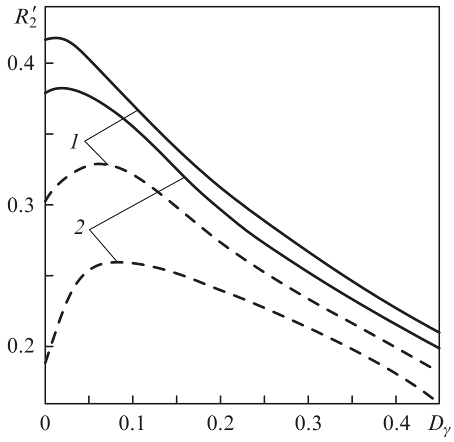


**Figure 3.** Dependence of diffuse reflectance $R'_2$ on $D_\gamma$ at $\lambda = 450$ (dashed curves) and 800 nm (solid curves) for $f_m$ = (*1*) 0.04 and (*2*) 0.16.

## 4. Conclusions

Diffuse reflectances of light are investigated using the probability density of slopes and the angular distribution function of micro areas. Selecting a specific assignment of the interface structure is determined by the convenience of calculations of double and triple integrals in the luminance factors of reflected (or refracted) light and the availability of relevant initial data. There are no specific differences between the two approaches, and in general they give similar values of diffuse reflectance for Gaussian and quasi-periodic surface models with equal slope variances. Analysis of the influence of shadowing effects on the integral reflection characteristics has shown that the screening of the incident and reflected beams by the relief elements is essential in the case of oblique incidence of the beam and, as a result, under diffuse illumination of the rough surface. Obviously, these effects also lead to a more significant decrease in diffuse reflectance with increasing slope variance. The effect of the angular illumination pattern on diffuse reflectance is studied under illumination of the inner surface of the stratum corneum by radiation multiply scattered in the tissue in-depth with refraction of the beam taken into account as it propagates to the interface with the surrounding medium. The significant impact of these factors on the integral characteristics of reflection is demonstrated.

To solve inverse problems of biomedical optics, i.e., to determine the structural and biophysical parameters of the tissue by the reflection spectra [11], the illumination pattern of the skin surface is easy to include in the corresponding algorithms. In this case, the diffuse reflectance $R'_2$ is the light characteristic, which is naturally included in the conditions of the problem statement, rather than a fitting parameter, as in

[11]. Note that the values of $R'_2$, calculated with the angular illumination pattern taken into account, lie already in the 'desired' range of 0.2–0.4 (Fig. 3), which depends on the wavelength. We can expect that this will improve the accuracy of recovery of the sought-for parameters of the skin. Peculiarities of the solution of the inverse problems of this type will be the subject of further research.

## Appendix

**Diffuse reflectance of a quasi-periodic rough surface in the case of an arbitrary angular illumination pattern**

Consider the reflection of light from a rough interface between two media with different refractive indices. Let us introduce the coordinate system $x'y'z'$ (Fig. A1). Near the boundary at point $O$ we select a micro area whose outer normal forms the angle $\beta'$ ($\pi/2 \leqslant \beta' \leqslant \pi$) with the $z$ axis and lies in the plane $x'z'$ (its azimuth is $\varepsilon = 0$). Let the beam with luminance $B(\psi,\phi)$ fall in the direction given by the polar ($\psi$) and the azimuth ($\phi$) angles, so that $0 \leqslant \psi \leqslant \pi/2$, $0 \leqslant \phi \leqslant 2\pi$. We determine the direction of the reflected beam by the angles $\chi'$, $\varphi$. Let the function $B(\psi,\phi)$ be symmetrical with respect to the plane $x'z'$. Then, to find the reflected light field it is sufficient to consider the range of azimuth angles of incidence $0 \leqslant \phi \leqslant \pi$, and to double the result obtained.

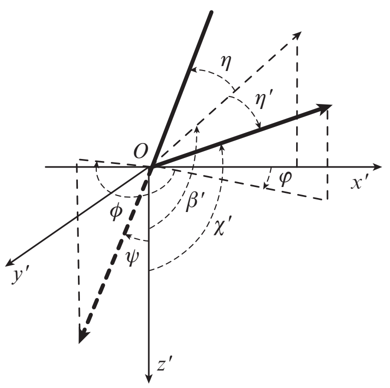


**Figure A1.** Coordinate system for calculating diffuse reflection on the basis of the angular distribution function of micro areas.

The equations of the plane of incidence and reflection in the coordinate system $x'y'z'$ have the form

$$\begin{vmatrix} x' & y' & z' \\ \sin\psi\cos\phi & \sin\psi\sin\phi & \cos\psi \\ \sin\beta' & 0 & \cos\beta' \end{vmatrix} = 0 \tag{A1}$$

and

$$\begin{vmatrix} x' & y' & z' \\ \sin\chi'\cos\varphi & \sin\chi'\sin\varphi & \cos\chi' \\ \sin\beta' & 0 & \cos\beta' \end{vmatrix} = 0. \tag{A2}$$

The angle $\eta$ of incidence is found as an additional angle to the normal formed by the incident beam with the coordinates ($\psi$, $\phi$) and direction ($\beta'$, 0):

$$\cos\eta = -\sin\psi\,\cos\phi\,\sin\beta' - \cos\psi\,\cos\beta'. \tag{A3}$$

The angle of reflection $\eta'$ is found similarly:

$$\cos\eta' = -\sin\chi'\cos\varphi\,\sin\beta' - \cos\chi'\cos\beta'. \tag{A4}$$

The angles $\psi$, $\phi$ and $\beta'$ are assumed specified, and $\chi'$ and $\varphi$ are unknown. Since the incident and reflected rays lie in one plane and the angle of incidence, $\eta$, equals the angle of reflection, $\eta'$, by equating the left-hand sides of (A1) and (A2), (A3) and (A4) we have a system of two equations for the two unknowns. Solving it with respect to $\chi'$, we obtain

$$\cos\chi' = -\cos\psi\,\cos 2\beta' - \sin\psi\,\cos\phi\,\sin 2\beta'. \tag{A5}$$

Here, as in [1–3], we take into account only single reflections of light from the surface relief elements. The angle $\chi'$, in this case, must satisfy the condition (Fig. A1)

$$\pi/2 \leqslant \chi' \leqslant \pi \ \text{ or } \ \cos\chi' \leqslant 0, \tag{A6}$$

and the angle $\eta$ – the condition

$$0 \leqslant \eta \leqslant \pi/2. \tag{A7}$$

These inequalities impose limitations on possible combinations of the angles $\psi$, $\phi$ and $\beta'$. Consider two cases.

(i) $\pi/2 \leqslant \beta' \leqslant 3\pi/4$ ($\cos 2\beta' \leqslant 0$ and $\sin 2\beta' \leqslant 0$). Then, to satisfy inequalities (A6), we derive from (A5) the limitation on the possible values of $\psi$, $\phi$ and $\beta'$:

$$-1 \leqslant \cos\phi \leqslant -1/(\tan\psi\,\tan 2\beta') \text{ at } 1/(\tan\psi\,\tan 2\beta') \geqslant 1 \tag{A8}$$

or which gives the last inequality from (A8),

$$\psi \geqslant 3\pi/2 - 2\beta \tag{A9}$$

and $\pi/2 \leqslant \phi \leqslant \pi$ at $1/(\tan\psi\tan 2\beta') < 1$.

(ii) $3\pi/4 \leqslant \beta' \leqslant \pi$ ($\cos 2\beta' \geqslant 0$ and $\sin 2\beta' \leqslant 0$). When $\cos\phi \leqslant 0$, (A6) holds true for any $\psi$ and $\beta$. When $\cos\phi > 0$, (A6) is fulfilled only at

$$\cos\phi \leqslant -1/(\tan\psi\,\tan 2\beta'). \tag{A10}$$

Note that there is one more limitation [apart from (A6)] for angles $\psi$, $\phi$ and $\beta'$. It is due to the fact that light must fall on micro area (*1*) from the 'desired' side (in the case of Fig. A1, from above). Mathematically, this limitation is written as $\cos\eta \geqslant 0$, or in the form of inequality (A7). From (A3) and (A4) it is easy to see that relationships (A8)–(A10) ensure fulfilment of this condition.

Thus, formulas (A3) and (A8)–(A10) give the necessary geometric relationship between the angles, allowing one to calculate the reflection coefficients $R$ and $R^*$ by the rough surface. Note that a similar problem was considered in [28] to study the structure of the light field reflected and refracted by a rough water surface. However, the final formula for $R$ has a typo {an extra factor $1/\cos\vartheta'$ in (A2.21) from [28]} and the limits of integration in $\psi$ and $\varphi$ are not presented. The latter is, probably, due to the fact that Mullamaa [28] considered a more complex situation of azimuth-dependent angular distribution of micro areas, and therefore the indicated limits of integration are more cumbersome. In this regard, the use of the known relations [28] without any mathematical calculations is difficult.

It was noted above that we calculate the reflection coefficients $R$ and $R^*$ of a quasi-periodic rough surface by using the concept of the angular distribution function $f(\beta)$ of micro areas. By definition [23] $f(\beta)$ is the area of micro areas whose normal is oriented within the solid angle $d\omega = \sin\beta d\beta d\varepsilon$ and which are projected onto the unit macro area. Obviously, the function $f(\beta)$ is normalised by the condition

$$2\pi\int_0^{\pi/2} f(\beta)\sin\beta\cos\beta d\beta = 1. \quad (A11)$$

Note that in (A11) $f(\beta)$ is assumed to be independent of the azimuth angle $\varepsilon$. In addition, the angular distribution function $F(\beta)$ of micro areas from [28] is related with the introduced [by (A11)] function [23] by the expression $F(\beta) = f(\beta)\times\cos\beta$. In the coordinate system shown in Fig. A1, $\beta = \pi - \beta'$.

Consider diffuse reflectance of light from a rough surface. The elementary flux incident on a macro area of unit area in a solid angle $d\omega_0 = \sin\psi d\psi d\phi$ has the form

$$d\Phi_0 = B(\psi,\phi)\cos\psi d\omega_0, \quad (A12)$$

and on micro areas of unit area –

$$d\Phi_1 = B(\psi,\phi)\cos\eta d\omega_0. \quad (A13)$$

The elementary flux reflected from micro areas whose normal is oriented within the solid angle is $d\omega_s = \sin\beta\, d\beta\, d\varphi$,

$$d\Phi_r = B(\psi,\phi)d\omega_0\cos\eta r_F(\eta)f(\beta)\sin\beta\, d\beta\, d\varphi. \quad (A14)$$

Diffuse reflectance $R'$ for an arbitrary angular illumination pattern $B(\psi,\phi)$ is by definition the ratio of the total reflected flux to the incident one. To calculate $R'$, one needs to integrate (A12) and (A14) in the angular coordinates:

$$R' = \frac{\int d\Phi_r}{\int_0^{2\pi} d\phi \int_0^{\pi/2} B(\psi,\phi)\cos\psi\sin\psi d\psi}. \quad (A15)$$

Taking into account the allowed values of the angles $\beta'$, $\psi$ and $\phi$, defined by (A8)–(A10), the numerator of (A15) takes the form

$$\int d\Phi_r = 4\pi\Bigg\{\int_{\pi/2}^{3\pi/4} f(\pi-\beta)\sin\beta d\beta \Bigg[\int_{3\pi/2-2\beta}^{\pi/2}\sin\psi d\psi \times\int_{\varkappa'}^{\pi}\cos\eta r_F(\eta)B(\psi,\phi)d\phi + \int_0^{3\pi/2-2\beta}\sin\psi d\psi \int_{\pi/2}^{\pi}\cos\eta r_F(\eta) \times B(\psi,\phi)d\phi\Bigg] + \int_{3\pi/4}^{\pi} f(\pi-\beta)\sin\beta d\beta\Bigg[\int_0^{\pi/2}\sin\psi d\psi \times\int_{\pi/2}^{\pi}\cos\eta r_F(\eta)B(\psi,\phi)d\phi + \int_0^{2\beta-3\pi/2}\sin\psi d\psi\int_0^{\pi/2}\cos\eta r_F(\eta) \times B(\psi,\phi)d\phi\int_{2\beta-3\pi/2}^{\pi/2}\sin\psi d\psi + \int_{\varkappa'}^{\pi/2}\cos\eta r_F(\eta)B(\psi,\phi)d\phi\Bigg]\Bigg\}, \quad (A16)$$

where $\varkappa' = \arccos[-1/(\tan\psi\tan 2\beta)]$.

Let us consider two particular cases of incidence of light on a rough surface. With directional illumination at the angle $\psi_0$ to the macro surface we can always assume that the azimuth of the incident beam is $\phi \equiv \phi_0 = 0$ or $\pi$ (depending on which side of the $z$ axis illumination occurs), and $B(\psi,\phi) = \delta(\cos\psi - \cos\psi_0)\delta(\phi - \phi_0)$ for a unit flux of the source. Substituting in (A15) and (A16), we obtain

$$R(\psi_0) = \frac{\pi}{\cos\psi_0}\bigg[ \int_{\pi/4}^{\pi/4+\psi_0/2} f(\beta)\cos(\beta-\psi_0)\sin\beta r_F(\beta-\psi_0)d\beta + \int_{\psi_0/2}^{\pi/4} f(\beta)\cos(\beta-\psi_0)\sin\beta r_F(|\beta-\psi_0|)d\beta + \int_0^{\pi/4-\psi_0/2} f(\beta)\cos(\beta+\psi_0)\sin\beta r_F(\beta+\psi_0)d\beta\bigg]$$

$$\text{at } \psi_0 \leqslant \pi/4,$$

$$R(\psi_0) = \frac{\pi}{\cos\psi_0}\bigg[ \int_{\psi_0}^{\pi/4+\psi_0/2} f(\beta)\cos(\beta-\psi_0)\sin\beta r_F(\beta-\psi_0)d\beta + \int_{\psi_0/2}^{\pi/4} f(\beta)\cos(\psi_0-\beta)\sin\beta r_F(\psi_0-\beta)d\beta + \int_0^{\pi/4-\psi_0/2} f(\beta)\cos(\beta+\psi_0)\sin\beta r_F(\beta+\psi_0)d\beta\bigg]$$

$$\text{at } \psi_0 > \pi/4. \quad (A17)$$

At normal incidence ($\psi_0 = 0$) we obtain (10). In the case of completely diffuse illumination, $B(\psi,\phi) = 1$, which yields formula (11). Note that (A16) does not take into account multiple reflections of light between micro areas and shadowing of incident and reflected rays by the elements of the surface relief. The latter effect can be easily introduced into (A16) as into (3), by multiplying the luminance $B(\psi,\phi)$ by the function $Q(a,b)$, where $b$, in the coordinate system shown in Fig. A1, is $\cot(\pi-\chi')/\langle\gamma_s\rangle$.

Thus, formulas (A15) and (A16) allow the calculation of diffuse reflectance of the rough surface at a known Fresnel reflection coefficient from a micro area, angular distribution functions of micro areas and angular distribution of the incident flux. Note that (A15) and (A16) yield the diffuse reflectance under irradiation of the surface by both polarised (at an arbitrary polarisation state) and unpolarised light.

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