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The accuracy of Kirchhoff's approximation in describing the far field speckles produced by random self-affine fractal surfaces

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Abstract. Based on the rigorous formulation of integral equations for the propagations of light waves at the medium interface, we carry out the numerical solutions of the random light field scattered from self-affine fractal surface samples. The light intensities produced by the same surface samples are also calculated in Kirchhoff's approximation, and their comparisons with the corresponding rigorous results show directly the degree of the accuracy of the approximation. It is indicated that Kirchhoff's approximation is of good accuracy for random surfaces with small roughness value w and large roughness exponent α. For random surfaces with larger w and smaller α, the approximation results in considerable errors, and detailed calculations show that the inaccuracy comes from the simplification that the transmitted light field is proportional to the incident field and from the neglect of light field derivative at the interface.

PACS. 42.25.Fx Diffraction and scattering – 42.30.Ms Speckle and moire patterns

1 Introduction

In the area of the diffraction and propagation of light waves, the Kirchhoff approximation (KA) is one of the most important theoretical methods and it predominates treatment of the problems pertinent to wave propagations due to its simplicity and convenience [1,2]. One category of these problems is the diffraction of light waves from regular and random medium interfaces. For regular interface, the diffracted field is also regular and then is comparatively simple, and the accuracy of KA has been widely proven in various optical systems, one example of which is the great success in designing the optical micro-device with a given intensity distribution by use of the inverse algorithm based on KA [3,4]. While the light waves are scattered from random surfaces, the intensity distributions are rather complicated and the speckles with granular appearances are usually formed [5–8]. Despite the overall applications of KA, the terms neglected or simplified such as the height derivatives of the random surface and the derivatives of the light field at the interfaces may have significant influences on the scattered light fields in the observation planes, and the accuracy of the approximation is not well understood. One of the difficulties therein is to relate practically a complicated speckle field to the surface profile producing it. Though at present, the height image of a random surface sample within a small specific area can be easily obtained with the scanning probe techniques (such as atomic force microscopy), such difficulty still exists because it is difficult to position exactly this area for illumination in an optical system and then to obtain its intensity distribution.

With the rapid development of both the near-field optics theories and the engineering of near-field optical microscopy, the accurate methods, such as the rigorous solutions of Green's integral equations [9–11] and the finite-difference time-domain (FDTD) method [12,13], have played more and more important roles in dealing with the light wave propagations. These methods make possible the connection of a random surface and its rigorous random light field by numerical implementations. Using the solutions of the Green's integral equations, Sanchez-Gil and Nieto-Vesperinas [9] have made the comparisons of the light scattering profiles of random surfaces which are the global average intensity distribution, with those obtained by KA. They have shown that the results by KA differ obviously from the accurate results. The local fluctuations in the intensity distributions, i.e., the speckles are more peculiar and are of more importance in either theoretical studies of light wave propagations or practical applications, and the studies on speckles have been recently extended to near-field case, where the KA is shown to be inappropriate. However, for the conventional far field

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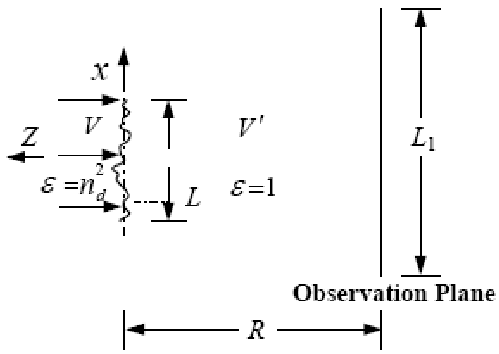

Fig. 1. The schematic diagram for light scattering at medium interface.

speckles, little work has been done on the fundamental problem that to what degree KA is accurate.

The self-affine fractal random surface is a model that can describe a variety of practical surfaces ranging from the material growth fronts to natural random screens [14,15]. In the growth process of thin film, the evolution of these parameters can reflect the mechanism of growth dynamics [14,16]. Moreover, recent studies [17,18] show that most natural random surfaces have obvious fractal characteristics, and can be more accurately characterized by self-affine fractal model than by the conventional one with Gaussian power spectrum. In this paper, we study the accuracy of the KA in the calculations of the speckle intensities produced by self-affine fractal random surfaces. The rigorous speckle intensities are computed by solving numerically the Green's integral equations at the random interface of medium. Comparing the rigorous results with the results obtained by KA, we find that KA is of good accuracy for random surfaces with small fluctuations, i.e., with small roughness w and large roughness exponent α, which is related to the fractal characteristics of the random surfaces. The speckle intensities of KA deviate obviously the rigorous results when surface roughness is increased. With detailed numerical verifications, we deduce that both the simplification for the light field on the random surface and the neglect of its derivative are the causes of inaccuracy of KA.

2 Theory

For the rigorous solutions of the speckle field, we start from the propagation of the light wave at a random interface of medium as shown in Figure 1. For simplicity, we assume a one-dimensional self-affine fractal random surface $z = D(x)$ separating a dielectric medium in the left half space $z > D(x)$ from vacuum in the right half space $z < D(x)$. An s-polarized parallel light wave $E^i(\boldsymbol{r})$ with a vacuum wavelength λ perpendicular to the coordinate plane $z = 0$ is incident on the surface from the dielectric medium, and here $\boldsymbol{r}$ is the position vector. Then the Helmholtz equations of light fields $E(\boldsymbol{r})$ and $E'(\boldsymbol{r})$ in the left and right half-spaces are, respectively:

$$\nabla^2 E(\boldsymbol{r}) + k^2 E(\boldsymbol{r}) = 0, \quad z > D(x), \quad (\boldsymbol{r} \in V) \tag{1a}$$

$$\nabla^2 E'(\boldsymbol{r}) + k_0^2 E'(\boldsymbol{r}) = 0, \quad z < D(x), \quad (\boldsymbol{r} \in V') \tag{1b}$$

where $k_0 = |\boldsymbol{k}_0| = 2\pi/\lambda$, $k = \sqrt{\varepsilon} k_0$. $E(\boldsymbol{r})$ and $E'(\boldsymbol{r})$ satisfy the following boundary conditions, respectively [9]:

$$E(\boldsymbol{r})\big|_{z=D^{(+)}(x)} = E'(\boldsymbol{r})\big|_{z=D^{(-)}(x)} \tag{2a}$$

$$\left[\frac{\partial E(\boldsymbol{r})}{\partial n}\right]_{z=D^{(+)}(x)} = \left[\frac{\partial E'(\boldsymbol{r})}{\partial n}\right]_{z=D^{(-)}(x)} \tag{2b}$$

where $D^{(+)}$ and $D^{(-)}$ represent approaching the interface $D(x)$ from the left and right half-spaces, respectively, and $\partial/\partial n = (\boldsymbol{n}\cdot\nabla)$ with $\boldsymbol{n} = (1/\gamma)\{-d[D(x)]/dx, 1\}$ and $\gamma = (1 + \{d[D(x)]/dx\}^2)^{1/2}$. In the left space $E(\boldsymbol{r})$ is the sum of the incident wave and the wave scattered from the surface. Applying Green's theorem to the Helmholtz equations (1a) and (1b), and with the boundary conditions (2a) and (2b), we can obtain the integral equation set for the light fields at the medium surface [9]:

$$E^{(i)}[x, D(x)] + \frac{1}{4\pi}\int_{-\infty}^{+\infty} dx' \left\{ E(x')\left[\frac{\partial G}{\partial z'} - D'(x')\frac{\partial G}{\partial x'}\right] - GF(x')\right\} = E(x) \tag{3a}$$

$$-\frac{1}{4\pi}\int_{-\infty}^{+\infty} dx' \left\{ E(x')\left[\frac{\partial G_0}{\partial z'} - D'(x')\frac{\partial G_0}{\partial x'}\right] - G_0 F(x')\right\} = 0 \tag{3b}$$

where $E(x)$ and $E(x')$ denote the light field on the surface, $G_0 = G_0(\boldsymbol{r};\boldsymbol{r}') = i\pi H_0^{(1)}(k_0|\boldsymbol{r} - \boldsymbol{r}'|)$ and $G = G(\boldsymbol{r};\boldsymbol{r}') = i\pi H_0^{(1)}\left\{[\varepsilon(\omega)]^{1/2} k_0 |\boldsymbol{r} - \boldsymbol{r}'|\right\}$ are, respectively, the two-dimensional Green's functions in an infinite vacuum and dielectric medium. Here $H_0^{(1)}$ is the zeroth-order Hankel function of the first kind, and $F(x)$ is related to the derivatives of the light field on the surface with respect to the normal by $F(x) = \gamma[\frac{\partial E(\boldsymbol{r})}{\partial n}]_{z=D(x)}$. The light field $E'(\boldsymbol{r})$ in the right half-space can be given:

$$E'(\boldsymbol{r}) = -\frac{1}{4\pi}\int_{-\infty}^{+\infty} dx' \left\{ E'(x')\left[\frac{\partial G_0}{\partial z'} - D'(x')\frac{\partial G_0}{\partial x'}\right] - G_0 F(x')\right\}, \quad (\boldsymbol{r} \in V'). \tag{4}$$

For the given the incident light field $E^i(\boldsymbol{r})$ and the height distribution $D(x)$ of the medium surface and with the light filed $E(x')$ and its derivative $F(x')$ at the boundary solved from integral equation set (3), the rigorous light field $E'(\boldsymbol{r})$ scattered from the surface can be calculated from equation (4).

In order to see more clearly the theoretical difference between the rigorous solution of the scattered light field $E'(\boldsymbol{r})$ and that of KA, we show in the following how the results of KA for the scattered field $E'(\boldsymbol{r})$ is obtained from equation (4). In KA, the light field $E'(x')$ immediately after the surface is simplified as the product of the incident light field $E^i(x')$ and the transmitted coefficient $T(x')$:

$$E'(x') = T(x')E^i(x') = T(x')\exp[-ikD(x')]. \quad (5)$$

In the calculation of $F(x')$, the Fresnel coefficient $T(x')$ is usually considered as the constant value at the normal incidence, i.e., $T(x') \approx T = 2n/(n+1)$, and the derivative with respect to the normal n is approximated as that to x:

$$F(x') = -ikTD'(x')\exp[-ikD(x')]. \quad (6)$$

Applying equations (5, 6) to equation (4), we have the light field $E'(\boldsymbol{r})$ in the right half-space:

$$E'(\boldsymbol{r}) = -\frac{T}{4\pi}\int_{-\infty}^{+\infty} dx'\exp[-ikD(x')]\left\{\left[\frac{\partial G_0}{\partial z'} - D'(x')\frac{\partial G_0}{\partial x'}\right] + ikD'(x')G_0\right\}. \quad (7)$$

Considering the argument $k_0|\boldsymbol{r} - \boldsymbol{r}'| = k_0\sqrt{(x-x')^2 + (z-z')^2} \gg 1$ in the one-dimensional Green's function G_0 in the Fresnel diffraction region and using the asymptotic expressions of Bessel and Neumann functions, we have:

$$G_0 = i\pi H_0^{(1)}(k_0|\boldsymbol{r} - \boldsymbol{r}'|) \sim i\pi\sqrt{2/\pi k_0\rho}\exp(ik_0\rho - i\pi/4) \quad (8)$$

$$\frac{\partial G_0}{\partial z'} - D'(x')\frac{\partial G_0}{\partial x'} = i\pi k_0\frac{(z-z') - D'(x')(x-x')}{\rho}H_1^{(1)}(k_0\rho) \sim i\pi k_0\frac{(z-z') - D'(x')(x-x')}{\rho}\sqrt{2/\pi k_0\rho}\exp(ik_0\rho - i3\pi/4) \quad (9)$$

and

$$k_0\rho = k_0\sqrt{(x-x')^2 + [z - D(x')]^2} \approx -k_0 z\left[1 - \frac{D(x')}{z} + \frac{(x-x')^2}{2z^2}\right]. \quad (10)$$

where $\rho = |\boldsymbol{r} - \boldsymbol{r}'|$, and the negative sign denotes the right half-spaces ($z < 0$). Another simplification made in KA is the "small slope approximation", with which derivative of the height distribution is neglected. Then substituting the above equations into equation (7), we obtain finally the expression in KA for the scattered light field $E'(\boldsymbol{r})$:

$$E'(x) = -i\frac{T}{4}\sqrt{2k_0/\pi\rho}\exp(-i3\pi/4)\exp(-ik_0 z) \times \int_{-\infty}^{+\infty} dx'\exp[-ik_0(n-1)D(x')]\exp[-ik_0(x-x')^2/2z]. \quad (11)$$

Except for the phase factor $\exp(-i3\pi/4)$, the above equation is same as the familiar expression for the light field in the Fresnel diffraction region produced by the random phase screen of $T\exp[-ik_0(n-1)D(x')]$ with the conventional Green's function $G_A(r) = \exp(ikr)/r$. Furthermore, if we replace the transmittance function of the phase screen by $R\exp\{-i[\boldsymbol{k}_{||}\cdot\boldsymbol{r}' + k_z D(x')\}$, with $\boldsymbol{k}_{||}$ and k_z the parallel and the perpendicular components of the wave vector, respectively, and R the reflectivity, equation (11) will become the scattered light field in the Fresnel diffraction for a reflectance object. With the further simplification the light field in the Fruanhofer diffraction region can be obtained.

3 Numerical implementation

For a random surface sample with given height distribution data, we first need to solve numerically the light field E and its derivative F at the medium boundary with equation set (3a) and (3b). For numerical solutions to be implemented, this integral equation set is discretized into the linear equation set [9–11]:

$$\begin{bmatrix} \boldsymbol{A}+\boldsymbol{I} & \boldsymbol{B} \\ \boldsymbol{A}^{(0)} - I & \boldsymbol{B}^{(0)} \end{bmatrix}\begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{F} \end{bmatrix} = 2\begin{bmatrix} \boldsymbol{E}^{(i)} \\ 0 \end{bmatrix} \quad (12)$$

where $\boldsymbol{I}$ is the identity matrix, and the (m,n) elements A_{mn}, B_{mn}, $A_{mn}^{(0)}$ and $B_{mn}^{(0)}$ of the $N \times N$ index matrices $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{A}^{(0)}$ and $\boldsymbol{B}^{(0)}$ are related to the surface height $D(x)$ and its first and second order derivatives, the Green's function $H_0^{(1)}(k_0|\boldsymbol{r} - \boldsymbol{r}'|)$ and its derivative $H_1^{(1)}(k_0|\boldsymbol{r} - \boldsymbol{r}'|)$, and so on. The detailed expressions of these matrix elements are given in reference [9]. Solutions of equation (12) will give the discretized light field E_n and its derivative F_n which are the elements of the vectors $\boldsymbol{E}$ and $\boldsymbol{F}$. Thus, the transmitted light field in the right half space can be calculated from equation (4).

For construction of the index matrices given in equation (12), the surface height distributions and their derivatives need to be first generated. In the paper, we use the self-affine fractal random surface as the model for the medium interface, whose morphological characteristics are described by its height-height correlation function [8,19]:

$$H_D(\rho) = \langle[D(x+\rho) - D(x)]^2\rangle = 2w^2\{1 - \exp[-(\rho/\xi)^{2\alpha}]\} \quad (13)$$

where $\langle\rangle$ denote the ensemble average, w is the root-mean-square roughness, ξ is the lateral correlation length and α is the roughness exponent relating to the fractal dimension d_f by $d_f = d - \alpha$, with d the embedded dimension. When $\alpha = 1$, the random surfaces have Gaussian correlation. We use the speckle-autocorrelation- function-analogy algorithm which we have proposed in reference [20] to generate self-affine fractal surfaces. To avoid the mathematical non-differentiatabilty of $D(x)$ due to the fractal characteristics of the surfaces, the first order and second order

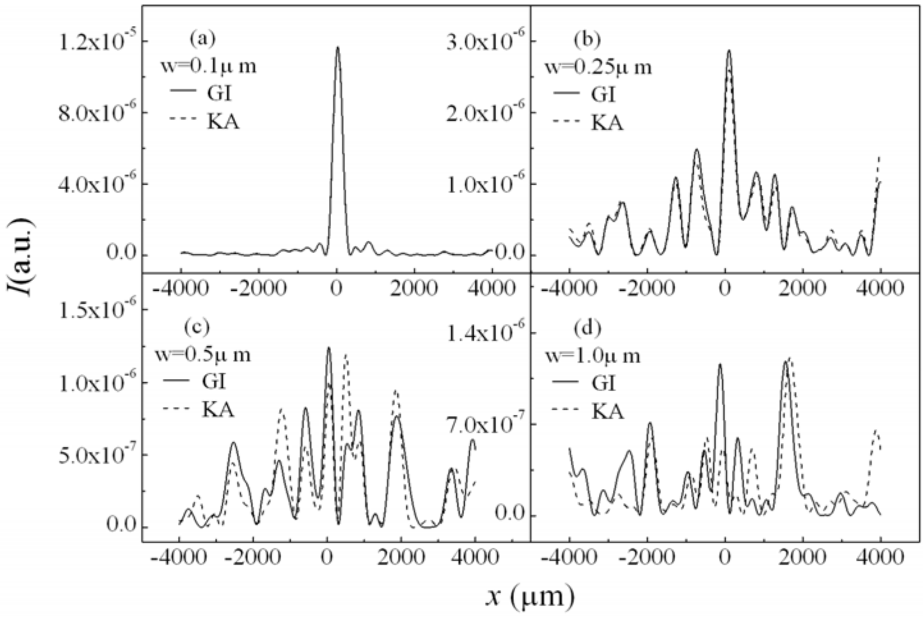

Fig. 2. The speckle intensities obtained by Green's integral (GI) equation (solid lines) and by KA (dash lines) with surface parameters $\alpha = 1.0$, $\xi = 0.5$ μm and $w = 0.1$, 0.25, 0.5, 1.0 μm ((a)–(d)), respectively.

derivatives, respectively, are calculated with the Fourier transform method:

$$dD(x)/dx = \int_{-\infty}^{+\infty} i2\pi f_x F_T(f_x) \exp(i2\pi f_x x) df_x \quad (14a)$$

$$d^2D(x)/d^2x = \int_{-\infty}^{+\infty} (i2\pi f_x)^2 F_T(f_x) \exp(i2\pi f_x x) df_x \quad (14b)$$

where $F_T(f_x)$ is the Fourier transform of $D(x)$.

In the practical numerical performance, the number N of the sampling points is 1000. The amplitude of the incident light is set unity. The refractive index $n = \sqrt{\varepsilon}$ of the medium is 1.532 corresponding to that of glass, and $\lambda = 632.8$ nm. The relationship $H_\nu^{(1)}(Z) = J_\nu(Z) + iY_\nu(Z)$ is used, with J_ν Bessel function and Y_ν Neumann function. When the argument Z is small ($Z < 0.1$) and large ($Z > 17.5$), the asymptotic expressions of these two functions are used; when Z takes medium values ($0.1 \leq Z \leq 17.5$), the values of these functions are input into the program with the increment of Z being 0.1, and then linear interception is used for calculation of the values of the functions at arbitrary Z. The linear equation set (12) is finally solved with Gaussian elimination, and thus E_n and F_n for the random surface sample are obtained, with which the scattered light field are directly calculated according to equation (4).

In contrast to the complicated above process of the rigorous solutions, the calculations of the scattered field of KA are rather simple. The light field $E'(\boldsymbol{r})$ is directly calculated based on equation (11) with height distribution $D(x)$ of random surface sample generated above.

4 Results and discussions

With the light field E_n and F_n for a random surface sample solved from the linear equation set (12), the rigorous intensity distribution of the speckle field at any distance from the near-field optical region to the far field diffraction regions can be obtained. In the recent work [21], we have shown that speckles exist on the random surface and in the near-field of the surface, and this phenomenon can not be appropriately described by KA. In order to understand the accuracy of KA for the speckles in far field diffraction regions, we now concentrate on rigorous calculations of speckle intensity $I(\boldsymbol{r}) = |E(\boldsymbol{r})|^2$ in these regions based on solutions of E_n and F_n, and then compare the results in detail with those of the KA. In the calculation, the lateral range L of random surfaces is set 20 μm, the lateral range of observation plane is $L_1 = 8$ mm and its distance from the random surface is $R = 1$ cm. The solid lines and dash lines in Figures 2a–2d, respectively, show the speckle intensity distributions obtained by rigorous solutions of Green's integral (GI) equations and by KA with surface parameters $\alpha = 1.0$, $\xi = 0.5$ μm and $w = 0.1$, 0.25, 0.5, 1.0 μm, respectively. The curves in Figures 3a–3d give intensity distributions under the same conditions as those in Figures 2a–2d, respectively, but with $\alpha = 0.6$. From the results in (a) and (b) of Figures 2 and 3, we can see that when the roughness w of the random surface is small, the speckle intensities obtained by KA are of little difference from the rigorous results by the Green's integral equation. This means that KA is of good accuracy for the calculation of the speckle field of random surfaces with small roughness values. With increase of the roughness of the random surface, as in (c) of both Figures 2 and 3, where the roughness is 0.5 μm, the intensity distributions of KA deviate greatly from the rigorous solutions of Green's integral equations. Furthermore, the curve by KA in Figure 3c deviates from the rigorous curve much

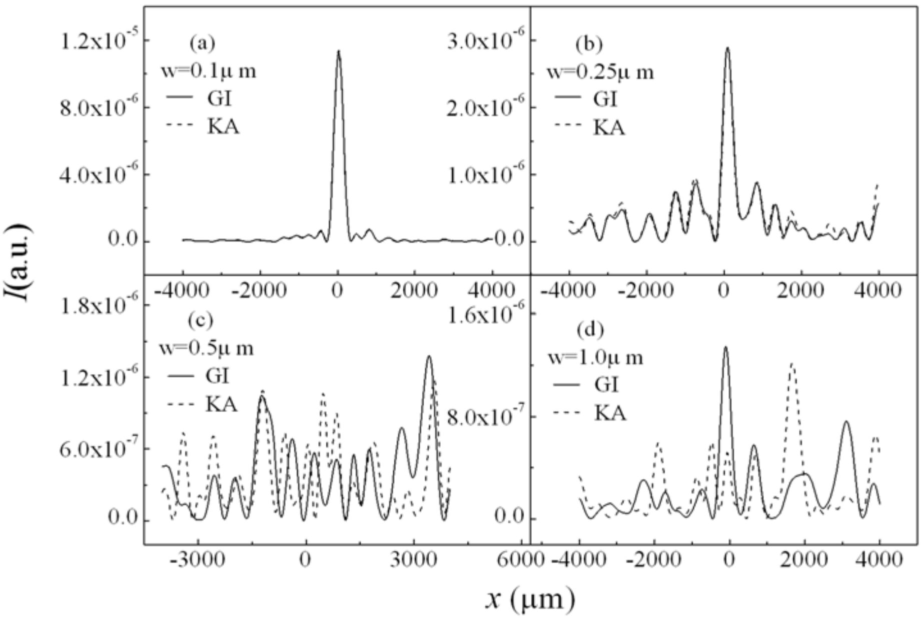

Fig. 3. The speckle intensities obtained by Green's integral (GI) equation (solid lines) and by KA (dash lines) with surface parameters $\alpha = 0.6$, $\xi = 0.5$ μm and $w = 0.1$, 0.25, 0.5, 1.0 μm ((a)–(d)), respectively.

more obviously than that in Figure 2c. This indicates that for the same value of roughness, KA is less accurate for the scattered light field from random surfaces with smaller α, i.e., with greater local fluctuations. For larger roughness of the surfaces ($w = 1.0$ μm), we see that in Figure 2d the intensity distribution by KA is very much different from the rigorous result though some resemblance still exists, and in Figure 3d the two intensity curves are totally different. This means that KA is very inaccurate or even invalid for the calculation of the speckle fields scattered from the random surfaces with large roughness.

To understand the essence of the inaccuracy of KA, we next consider in detail properties of light field E_n on the surface, its derivative F_n, the derivative of surface height $D'(x)$ and the Green's function and their influences on the scattered light field by rigorous calculation. For each surface sample, we first obtain the rigorous light field E_n and the derivative F_n by solving equation (12), and then calculate scattered light intensity according to equation (4) in different cases. Figures 4a–4d give the results for surface samples with $\xi = 0.5$ μm and $\alpha = 0.6$. In Figure 4a, the solid curve is the intensity distribution calculated based on equation (4) with F_n and $D'(x)$ neglected, and the dash curve is directly obtained from equation (11). Since in the calculations of them, the Green's functions are the same and light fields on surface are the rigorous E_n and the $E'(x')$ of KA given in equation (5), respectively, the difference of these two curves shows that the degree of inaccuracy with $E'(x')$ in equation (5) as the surface light field in KA is rather significant.

Figure 4b gives the intensity curves to compare the influences of the derivatives. The dash curve is the rigorous scattered intensity calculated based on equation (4), and the dash dot curve and solid one are also calculated according equation (4), but with the derivative F_n of light field and with both F_n and the derivative $D'(x)$ of the surface height neglected, respectively. We note here that the solid curve is the same as the solid one in Figure 4a. The little difference in the dash dot curve and solid one shows the derivative of the surface height $D'(x)$ in equation (4) contribute little to the scattered field. Then comparing the dash dot curve with the rigorous result dash curve, we may see from the great difference in them that the derivative F_n is of great influence on the intensity distribution. This indicates that the simplification of equation (6) in KA for the derivative of the light field on the surface, which originates in essence from equation (5) and simplified to be proportional to the light field itself, is very much inaccurate.

Figures 4c and 4d show the rigorous intensities and the intensities calculated with the derivatives F_n and $D'(x)$ neglected for random surface samples with roughness values $w = 0.25$ μm and $w = 0.5$ μm, respectively. We see that the larger the roughness of random surfaces is, the greater the errors will be induced by neglecting the derivatives F_n.

To verify the above conclusions for the light fields on observation planes with farther distance from the random surface, we also calculate the speckle intensities with distance $R = 20$ cm, and the same conclusions as above can be reached.

It should be noted that equation (11) is the small slope approximation to KA. Rigorously speaking, in KA the Fresnel transmission coefficient at a point on the random surface depends the local angle of incidence, which is related to the local slope $D'(x')$. It is well understood that the consideration of $D'(x')$ will make the analytical manipulation of KA for scattering problem very complicated. The majority of the literature neglects $D'(x')$ for simplicity and uses equation (11) for the calculation of scattered light field [1]. Then making clear the difference of its results from those of the rigorous solution of the Green's

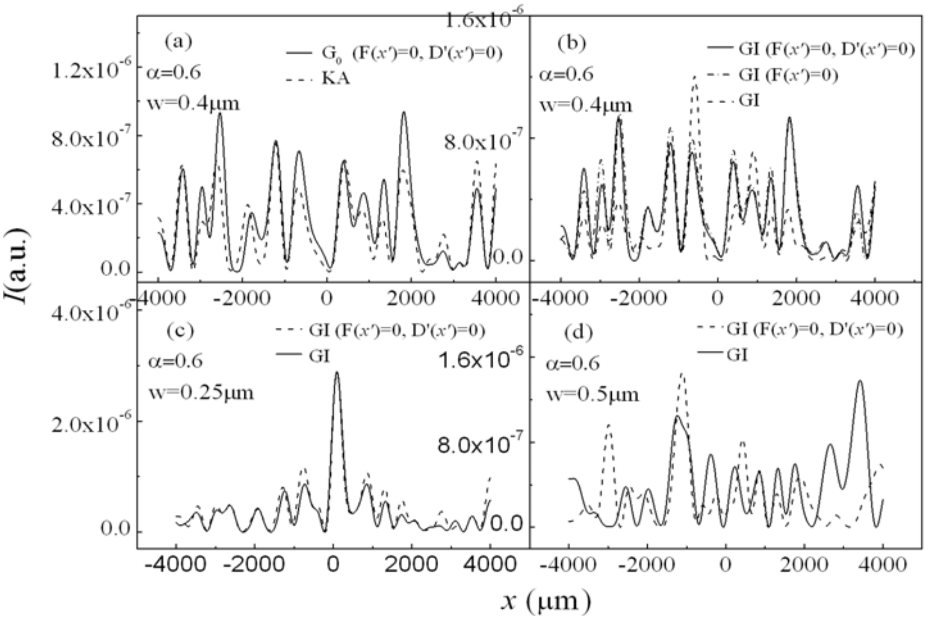

Fig. 4. (a) Gives the intensities calculated based on equation (4) with neglect of F_n and $D'(x)$ (solid curve) and directly obtained by KA (dash curve), respectively. (b) The comparisons of the rigorous intensity (dash curve) with those calculated with F_n neglected (dash dot curve) and both F_n and $D'(x)$ neglected (solid curve), respectively. (c) and (d) The comparisons of the rigorous intensities with those given by neglecting both $F(x)$ and $D'(x)$ with roughness $w = 0.25$, 0.5 μm, respectively.

integral equation is necessary, and this is what this paper is actually aimed to. In addition, $D'(x')$ diverges mathematically due to the fractality of surfaces. However, from the viewpoint of physics, the fractality of random surfaces is limited to a reasonable spatial range rather than extending to that from the infinitively small to the infinitively large, and hence $D'(x')$ may be physically regarded as finite. Indeed, $D'(x')$ may become very large due to the fractality, but the results in Figure 4b indicate that the solid intensity curve with neglect of both F_n and $D'(x')$ is still close to the dash dot curve with mere neglect of F_n, though some minor errors do exist. This may justify the necessity of studying the accuracy the KA with the slope of the surface neglected.

5 Conclusion

Starting from the Green's integral and Kirchhoff's approximation, we calculate the rigorous and the approximate speckle intensities produced by the self-affine random surface, respectively. We study the accuracy of KA for calculation of light field by comparing the rigorous results with those obtained by KA. It is found that the accuracy of KA depends on the surface parameters roughness value w and the roughness exponent α, i.e., KA has high accuracy for the surfaces with small w and large α and vice versa. From the detailed comparisons of the intensities in different cases, we draw a conclusion that both the simplification for the light field on the random surface and the neglect of its derivative cause the inaccuracy of KA.

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