Half-width of intensity profiles of light scattered from self-affine fractal random surfaces and simulational verifications

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Based on the fact that the half-width of the Fourier transform is inversely proportional to that of a symmetrical primary decay function, the half-width of the intensity profiles of light scattered from self-affine fractal random surfaces in the whole $k_\perp$ region is studied. The primary function, whose Fourier transform is the intensity profile, is approximated with a simple mathematical decay function by equating their half-widths and maximums. The expression obtained for the half-width of the scattered intensity profiles reduces to the present results in the two extreme cases with the scattering roughness factors being either very small or very large. For a complete verification, we perform a simulation of the light scattering, in which self-affine fractal random surfaces are generated with an algorithm that is an analogy to the formation of laser speckles. The simulated and theoretical results conform well.

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I. INTRODUCTION

The self-affine fractal random surface is a model that can describe many practical surfaces ranging from the material growth fronts [1,2] to natural random screens [3,4]. The parameters of random surfaces of this kind include the root-mean-square deviation roughness w, the lateral correlation length ξ, and the roughness exponent α that shows the fractal properties of the surfaces. It is well known that the scattering technique is one of the most powerful tools for random surface characterizations, and its applications to self-affine fractal random surfaces are of great interest [5–10]. Yang *et al.* [11,12] have come up with the theoretical results of scattering from self-affine fractal surfaces, in which one of the most interesting and useful results is the full width at half maximum of the scattered intensity profiles when the scattering roughness factor $\Omega = k_\perp^2 w^2$ is either very small or very large. Based on these results, a light scattering scheme with varied angles of incidence is developed [9,10,13], with which one can extract the lateral correlation length ξ and the roughness exponent α of a random surface sample from the measured intensity profiles corresponding to different incident angles of the illuminating light beam. This to some degree breaks free from the limitations of the conventional scattering method that usually uses a single profile at a certain angle of incidence for extraction of the surface parameters. When the scattering roughness factor Ω takes medium values, the corresponding incident angles of the illuminating light beam often have moderate values, and therefore the measurements are more convenient and easier to perform. However, to our knowledge, how the half-width of the scattered profiles with medium Ω behaves and how it is related to the surface parameters is not well understood, and therefore, the method for extraction of surface parameters from the widths of the measured profiles in the corresponding incident angles has not been developed.

Based on the principle that the half-width of the Fourier transform of a symmetrical decay function is inversely proportional to the half-width of the function itself, and by approximating with a simple mathematical decay function the primary function whose Fourier transform is the intensity profile, we derive a generic expression for the half-width of the intensity profiles scattered from self-affine fractal random surfaces. As Ω takes either very small or very large values, this expression reduces to the present results for both the extreme cases. For the complete verification of this generic expression, we propose a method for generation of self-affine fractal random surfaces by an analogy of surface height to laser speckle fields, and simulate its light scattering, with the intensity profiles obtained at different angles of incidence. The variation of the half-width of these simulated profiles versus the perpendicular component of the wave vector conforms well with that predicted by the expression of this paper. The results of this paper promise the method for extraction of surface parameters from the profiles of the medium Ω region.

II. THE HALF-WIDTH OF THE SCATTERING PROFILES AT $\Omega \ll 1$ AND $\Omega \gg 1$

The autocorrelation function of the height $h(\boldsymbol{r}_0)$ of a self-affine fractal function can be characterized by the following phenomenological function [7,12]:

$$R_h(\boldsymbol{\rho}) = \langle h(\boldsymbol{r}_0) h(\boldsymbol{r}_0+\boldsymbol{\rho})\rangle = w^2 \exp[-(\rho/\xi)^{2\alpha}], \qquad (1)$$

where $\boldsymbol{r}_0$ is the position vector, $\rho = |\boldsymbol{\rho}|$, and the roughness exponent α is related to the surface fractal dimension D_f by $\alpha = d - D_f$ with $0 \leqslant \alpha \leqslant 1$ and d being the embedded dimension. More often, another choice, i.e., height-height correlation $H(\boldsymbol{\rho})$, is used for characterizing the random surfaces. It is defined as

$$H(\boldsymbol{\rho}) = \langle [h(\boldsymbol{r}_0+\boldsymbol{\rho}) - h(\boldsymbol{r}_0)]^2\rangle = 2[w^2 - R_h(\boldsymbol{r}_0, \boldsymbol{r}_0+\boldsymbol{\rho})]. \qquad (2)$$

According to Kirchhoff's theory of diffraction, when the random surface is illuminated by an incident light wave with wavelength λ_0 and wave vector $\boldsymbol{k}_0$, the scattered wave corresponding to wave vector $\boldsymbol{k}$ is

$$U(\boldsymbol{k})=\int \exp[-ik_\perp h(\boldsymbol{r}_0)]\exp(-i\boldsymbol{k}_\parallel\cdot\boldsymbol{r}_0)d^2\boldsymbol{r}_0, \tag{3}$$

where $\boldsymbol{k}=\boldsymbol{k}_s-\boldsymbol{k}_0$, $\boldsymbol{k}_s$ is the wave vector of the scattered wave, $\boldsymbol{k}_\perp$ and $\boldsymbol{k}_\parallel$ are the perpendicular and parallel components of $\boldsymbol{k}$, respectively, $k_\perp=2\pi\cos\theta(1+\cos\beta)/\lambda \approx 4\pi\cos\theta/\lambda$, and $k_\parallel=2\pi\sin\beta/\lambda$, with θ and β representing, respectively, the angle of incidence and the angle between the scattered wave vector and the direction of the specular reflection. The scattered intensity profile can be written as [8]

$$I(\boldsymbol{k})=\langle U(\boldsymbol{k})U^*(\boldsymbol{k})\rangle=\int_{-\infty}^{+\infty}\exp[-k_\perp^2H(\boldsymbol{\rho})/2]\times\exp(-i\boldsymbol{k}_\parallel\cdot\boldsymbol{\rho})d^2\boldsymbol{\rho}. \tag{4}$$

For the self-affine fractal random surfaces whose height-height correlation $H(\boldsymbol{\rho})$ is given by Eq. (1) and Eq. (2), it is impossible to obtain from the above equation the rigorous solution of $I(\boldsymbol{k})$ as the explicit non-integral-transform function of $\boldsymbol{k}$. Therefore, approximations should be taken into account for further simplification of $I(\boldsymbol{k})$. Yang *et al.* [11,12] have proved that when the scattering roughness factor $\Omega=k_\perp^2w^2\ll 1$, $I(\boldsymbol{k})$ is expressed by

$$I(\boldsymbol{k})=I(k_\parallel)=(2\pi)\exp(-k_\perp^2w^2)\left[2\pi\delta(k_\parallel)+k_\perp^2w^2\xi^2\int_0^\infty\exp(-t^{2\alpha})tJ_0(k_\parallel\xi t)dt\right], \tag{5}$$

while when $\Omega=k_\perp^2w^2\gg 1$, $I(\boldsymbol{k})$ is expressed by

$$I(\boldsymbol{k})=I(k_\parallel)=\xi^2(k_\perp w)^{-2/\alpha}\times\int_0^\infty\exp(-t^{2\alpha})tJ_0(k_\perp^{-1/\alpha}w^{-1/\alpha}\xi k_\parallel t)dt. \tag{6}$$

The first term on the right-hand side of Eq. (5) represents the central δ peak in the scattered profile, which is caused by the specular reflection. The diffused terms represented by the integrals in both Eq. (5) and Eq. (6) are the Bessel-Fourier transforms of $\exp(-t^{2\alpha})$, which remain analytically unsolvable except for $\alpha=1$. However, it is sure that they are symmetrical decay functions of $k_\parallel$ with the arguments being $k_\parallel\xi$ and $k_\perp^{-1/\alpha}w^{-1/\alpha}\xi k_\parallel$, respectively, for $\Omega\ll 1$ and $\Omega\gg 1$. Therefore, the half-widths of these two functions are inversely proportional to the coefficients of $k_\parallel$ in the arguments

$$W_p\propto\begin{cases}1/\xi, & \Omega\ll 1,\\ [k_\perp^{-1/\alpha}w^{-1/\alpha}\xi]^{-1}, & \Omega\gg 1.\end{cases} \tag{7}$$

We can further obtain the equality expressions for the proportional relations by using the width of the scattering profiles with roughness exponent $\alpha=1$. In this case, the primary function $\exp(-t^{2\alpha})$ in the Fourier transform in Eq. (5) and Eq. (6) turns into $\exp(-t^2)$. Then, from the properties of the integral of Bessel function, we have

$$F(k_\parallel)=\int_0^\infty\exp(-t^2)tJ(\xi k_\parallel t)dt=\frac{1}{2}\exp[-(k_\parallel\xi/2)^2]. \tag{8}$$

By defining the half-width of $F(k_\parallel)$ as the $k_\parallel$ value which $F(k_\parallel)$ drops to $1/e$ of its maximum, we obtain from Eqs. (5), (6), and (8) that when $\alpha=1$ the half-widths W_p of the scattered profiles are $2/\xi$ and $2/(k_\perp^{-1}w^{-1}\xi)$, respectively, for the two extreme cases. This determines that the proportionality coefficients in expression (7) should be 2. Thus we have the width of the scattering profiles for the arbitrary α:

$$W_p=\begin{cases}2/\xi, & \Omega\ll 1,\\ 2/(k_\perp^{-1/\alpha}w^{-1/\alpha}\xi), & \Omega\gg 1.\end{cases} \tag{9}$$

III. THE HALF-WIDTH OF THE SCATTERING PROFILES FOR ARBITRARY Ω

In order to obtain the expression for the half-width of the profile $I(\boldsymbol{k}_\parallel)$ at arbitrary $\Omega=k_\perp^2w^2$, we rewrite $I(\boldsymbol{k}_\parallel)$, from Eqs. (1), (2), and (4), as

$$I(\boldsymbol{k}_\parallel)=(2\pi)^2\exp(-\Omega)\delta(\boldsymbol{k}_\parallel)+I_{\text{diff}}(\boldsymbol{k}_\parallel,k_\perp). \tag{10}$$

The first term on the right-hand side of the above equation represents the central δ peak, and the second term is the diffused term

$$I_{\text{diff}}(\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp)=I_{\text{diff}}(\boldsymbol{k}_\parallel)=2\pi\exp(-\Omega)\xi^2\times\int_0^\infty\{\exp[\Omega\exp(-x^{2a})]-1\}xJ_0(k_\parallel\xi x)dx. \tag{11}$$

In the Fourier transform on the right-hand side of the above equation, the primary function that we represent by $G(x)=\exp[\Omega\exp(-x^{2\alpha})]-1$ is a symmetrical decay function of x with $[\exp(\Omega)-1]$ its maximum at $x=0$, and zero its minimum as $x\to\infty$. If we analytically fit it using the simple decay functions $D(x)$, such as Gaussians and Lorentzians, the half-width of the Fourier transform of the obtained $D(x)$ can be approximately taken as the half-width of that of $G(x)$. Thus we can get the half-width of the scattered profile $I_{\text{diff}}(\boldsymbol{k}_\parallel)$.

In order to choose $D(x)$, we have tried several mathematical decay functions to fit $G(x)$ and found the best one is

$$D(x)=B\exp[-(x/A)^{2\alpha}], \tag{12}$$

with its form being the closest to that of $G(x)$ as well. The basic principle for the determination of the constants A and B in $D(x)$ is to let $D(x)$ and $G(x)$ have the same maximum at $x=0$ and the same half-width. Therefore, B should satisfy

$$B=G(0)=\exp(\Omega)-1, \tag{13}$$

and the half-width A of $D(x)$ should be the value of x at which $G(x)$ drops to $1/e$ of its maximum, which is expressed as

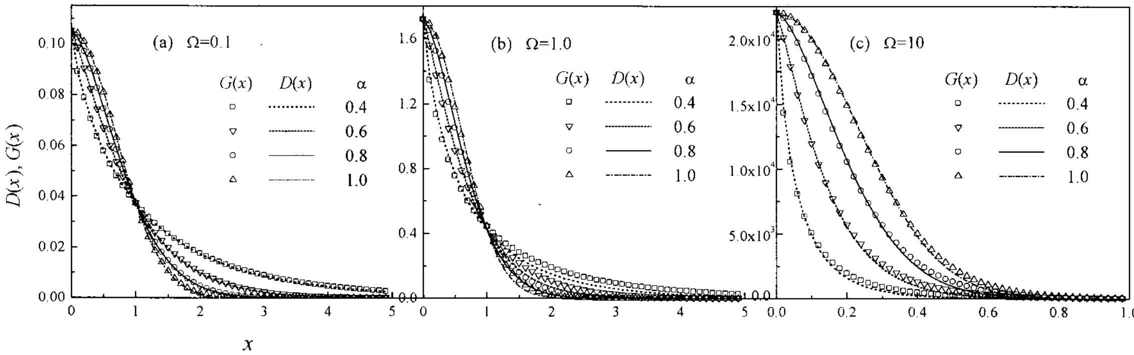

FIG. 1. The comparison of $G(x)$ and $D(x)$. (a) $\Omega=0.1$, (b) $\Omega=1.0$, and (c) $\Omega=10.0$.

$$\exp[\Omega\exp(-A^{2\alpha})]-1=[\exp(\Omega)-1]/e. \tag{14}$$

Then A is given by

$$A=\left\{\ln\frac{\Omega}{\ln[\exp(\Omega-1)+1-1/e]}\right\}^{1/2\alpha}. \tag{15}$$

Figure 1 shows the plots of $G(x)$ at different w and α values and those of the corresponding $D(x)$ with A and B calculated through the expressions (13) and (15). We see that the replacement of $G(x)$ with $D(x)$ is of good accuracy. Replacing $G(x)$ in Eq. (11) by $D(x)$, we have the approximate expression for the scattered profile,

$$\begin{aligned}I_{\rm diff}(\boldsymbol{k}_\parallel)&=2\pi\exp(-\Omega)\xi^2\int_0^\infty[\exp(\Omega)-1]\\&\quad\times\exp[-(x/A)^{2\alpha}]xJ_0(k_\parallel\xi x)dx\\&=2\pi A^2\xi^2\exp(-\Omega)[\exp(\Omega)-1]\\&\quad\times\int_0^\infty\exp(-x^{2\alpha})xJ_0(k_\parallel\xi Ax)dx.\end{aligned} \tag{16}$$

Referring to the derivation of expression (9) for W_p from Eqs. (5) and (6) in both the extreme cases, we can obtain from Eq. (16) the half-width W_p for arbitrary value of Ω,

$$W_p=2/(\xi A)=2\xi^{-1}\left\{\ln\frac{\Omega}{\ln[\exp(\Omega-1)+1-1/e]}\right\}^{-1/2\alpha}. \tag{17}$$

The detailed behavior of the approximate profile function $I_{\rm diff}(\boldsymbol{k}_\parallel)$ in Eq. (16) may differ to a certain degree from that of the rigorous profile $I_{\rm diff}(\boldsymbol{k}_\parallel)$ in Eq. (11), but their half-widths, which are what we are really concerned with here in this paper, should differ to a much less degree. Therefore, though derived from the approximate profile function, expression (17) for the half-width W_p is of good accuracy, as will be depicted in the following. Now we first discuss it in the two extreme cases. In Eq. (15), the term $\exp(\Omega-1)-1/e\approx\Omega/e\ll1$ as $\Omega\ll1$, and then we have

$$A\approx\left[\ln\frac{\Omega}{\ln(\Omega/e+1)}\right]^{1/2\alpha}\approx\left[\ln\frac{\Omega}{(\Omega/e)}\right]^{1/2\alpha}=1.$$

This reduces Eq. (17) to the result of Eq. (9),

$$W_p=2/\xi\quad(\Omega\ll1). \tag{18}$$

If we substitute $A=1$ into Eq. (16), our approximate expression (16) for the diffused profile turns into the diffused term in Eq. (5). When $\Omega\gg1$, Eq. (15) can be written as

$$A\approx\left\{\ln\frac{\Omega}{\ln[\exp(\Omega-1)]}\right\}^{1/2\alpha}=\left[\ln\left(1+\frac{1}{\Omega-1}\right)\right]^{1/2\alpha}\approx\Omega^{-1/2\alpha}.$$

Then Eq. (17) becomes

$$W_p=2/(\xi A)\approx2\xi^{-1}k_\perp^{1/\alpha}w^{1/\alpha}\quad(\Omega\gg1).$$

This is also the result in Eq. (9). In this case, if we substitute A into Eq. (16) and notice that $\exp(\Omega-1)\to\exp(\Omega)$ and that in Eq. (10), $\exp(-\Omega)\to0$, our approximate profile function $I_{\rm diff\alpha}(\boldsymbol{k}_\parallel)$ in Eq. (16) reduces exactly to Yang *et al.*'s results of Eq. (6). These coincidences partly verify the results of this paper. One may notice how simple the complicated mathematical process for the simplification of $I(\boldsymbol{k})$ to Eq. (6) turns out to be as illustrated in this paper.

IV. THE ALGORITHM FOR THE SURFACE GENERATION AND THE SIMULATION OF LIGHT SCATTERING

We now make use of the simulation technique of light scattering for a complete verification of Eq. (17). We first need an algorithm for the numerical generation of self-affine fractal random surfaces. Considering that the autocorrelation function $R_h(\rho)=w^2\exp[(-\rho/\xi)^{2\alpha}]$ is symmetrically decayed, and that its Fourier transform should be real and nonnegative, we define the function $p(\boldsymbol{u})$ by

$$\begin{aligned}p(\boldsymbol{u})&=[P(\boldsymbol{u})]^{1/2},\\P(\boldsymbol{u})&=\int_{-\infty}^{+\infty}w^2\exp[-(v/\xi)^{2\alpha}]\exp(i2\pi\boldsymbol{u}\cdot\boldsymbol{v})d^2\boldsymbol{v}.\end{aligned} \tag{19}$$

We call $p(\boldsymbol{u})$ the "aperture function" by analogy to the laser speckle theory [14]. The following expression is used for the generation of complex height distribution:

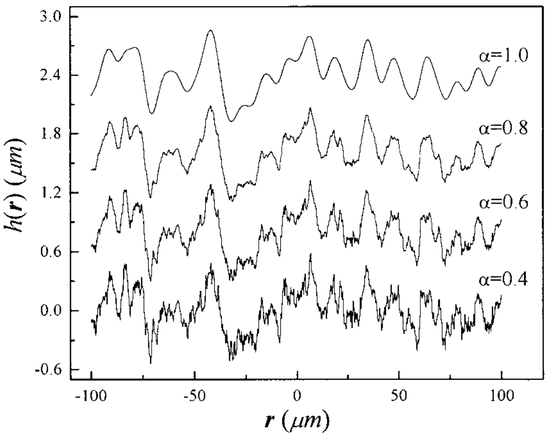

FIG. 2. The four surface samples generated with the same series of random number. To avoid overlap, background bases of 2.4, 1.6 and 0.8 μm are added, respectively, to samples with $\alpha=1.0$, 0.8, and 0.6.

$$h_c(\boldsymbol{r}_0)=h_r(\boldsymbol{r}_0)+ih_i(\boldsymbol{r}_0)$$
$$=\sqrt{2}\int_{-\infty}^{\infty}p(\boldsymbol{u})\,\eta(\boldsymbol{u})\exp(-i2\pi\boldsymbol{u}\cdot\boldsymbol{r}_0)d\boldsymbol{u}, \quad (20)$$

where $\eta(\boldsymbol{u})$ is a white-noise random process with zero-mean value, i.e., $\langle\eta(\boldsymbol{u})\rangle=0$ and $\langle\eta(\boldsymbol{u})\eta(\boldsymbol{u}')\rangle=\delta(\boldsymbol{u}-\boldsymbol{u}')$; $h_r(\boldsymbol{r}_0)$ and $h_i(\boldsymbol{r}_0)$ are, respectively, the real and imaginary parts of $h_c(\boldsymbol{r}_0)$. Following the way for studying the properties of the speckle light field [14], one will not find it too difficult to show that the autocorrelation functions of both $h_r(\boldsymbol{r}_0)$ and $h_i(\boldsymbol{r}_0)$ equal the one given in Eq. (1), and $h_r(\boldsymbol{r}_0)$ and $h_i(\boldsymbol{r}_0)$ are Gaussian random process with zero mean. Then both $h_r(\boldsymbol{r}_0)$ and $h_i(\boldsymbol{r}_0)$ can be taken as the height distribution of a self-affine fractal surface. In our practical computation, we use the numerically generated white-noise series for $\eta(\boldsymbol{u})$, and use only $h_r(\boldsymbol{r}_0)$ as the generated surface height, discarding $h_i(\boldsymbol{r}_0)$. In Fig. 2, four surface samples generated with the same series of $\eta(\boldsymbol{u})$ with $w=0.2$ μm, $\xi=6.0$ μm but different α values are shown. Next, the light field $U(\boldsymbol{k})=U(\boldsymbol{k}_\parallel)$ scattered at certain angle of incidence θ can be computed numerically based on Eq. (3), in which $k_\perp\approx 4\pi\cos\theta/\lambda$. λ is

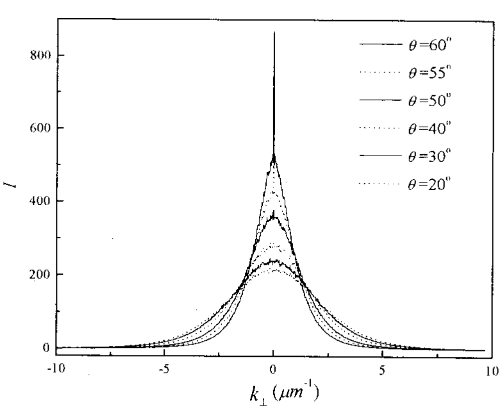

FIG. 3. Some of the scattered intensity profiles of surface ensemble 1.

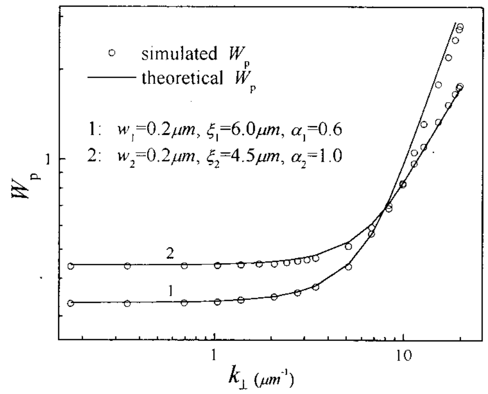

FIG. 4. The half-width of the scattered intensity profile versus $k_\perp$ for surface ensembles 1 and 2.

set to be 0.6328 μm, corresponding to the wavelength of He-Ne laser. With different series of $\eta(\boldsymbol{u})$ and unchanged values of parameters w, ξ, and α, we generate 4000 surface samples and take them as one surface ensemble. Arithmetically averaging all the intensities $I_u(\boldsymbol{k}_\parallel)=U(\boldsymbol{k}_\parallel)U^*(\boldsymbol{k}_\parallel)$ at the same $k_\parallel$ point produced by each of the surface samples in the ensemble, we obtain the ensemble average intensity $I(\boldsymbol{k}_\parallel)=\langle I_u(\boldsymbol{k}_\parallel)\rangle=\langle U(\boldsymbol{k}_\parallel)U^*(\boldsymbol{k}_\parallel)\rangle$. Then the simulated scattered profile can be readily obtained by calculating the $I(\boldsymbol{k}_\parallel)$ at all $k_\parallel$ points. For simplicity and lucidity, we only generate the one-dimensional random surfaces and simulate their scattered intensity profiles.

Figure 3 shows some of our simulated profiles at different angles of incidence, scattered by surface ensemble 1 with its parameters set at $w_1=0.2$ μm, $\xi_1=3.0$ μm, and $\alpha_1=0.6$. We see that the widths of the profiles increase as $k_\perp$ increases, or equivalently θ decreases, and the central δ peak appears when $k_\perp$ is small.

For one surface ensemble, we select 18 angles of incidence in the angle range from 0° to 90°, at each of which the corresponding scattered profile is simulated. Then by fitting each of the profiles with Gaussian function $G_f(x)=C\exp[-(k_\parallel/D)^2]$, we obtain the value of the constant D, which is taken as the half-width W_p of the simulated profile. This method for extracting the half-width of the scattered profiles has been used in the literature [10,13,15] and is shown to be effective and accurate enough. In Fig. 4, the half-widths of the simulated profiles produced by surface ensembles 1 and 2 are plotted versus $k_\perp$ in the log-log scale. Surface ensemble 2 is generated with parameters set at $w_2=0.2$ μm, $\xi_2=3.0$ μm, and $\alpha_2=1.0$. Figure 4 also shows in solid lines the W_p-$k_\perp$ curves obtained by substituting the parameters of the two surface ensembles into Eq. (17). It can be seen that the half-width expression of this paper conforms well to the results of simulation in the whole range of $k_\perp$.

V. CONCLUSIONS

We have studied the properties of the half-width of the intensity profiles of light scattered from the self-affine fractal random surfaces in the whole range of $k_\perp$. The introduction of the approximations for the primary function $G(x)$ makes it feasible to perform a theoretical analysis of the half-widths of the scattered intensity. The expressions we obtained give a full understanding of the behaviors of half-widths with the variation of incident angle of the light wave. The results obtained in the previous literature for $\Omega \ll 1$ and $\Omega \gg 1$, whose derivations were rather complicated, are included in our expressions and are obtained easily. Since the conclusion of this paper relates the half-widths of the profiles to all the statistical parameters of self-affine fractal random surfaces, it will be of great importance for practical measurements in experimental setups of light scattering with variable angles of incidence. The half-widths of the intensity profiles in the case of medium Ω, which is much more often met in experiments than the two extreme cases can be readily used for the surface parameters to be extracted. We believe that this will not only enlarge the measurable range of the random surface parameters with the scattering technique, but also greatly ease the experimental work. Besides, the algorithms proposed in this paper for the generation of self-affine fractal random surfaces and for their light scattering simulation will be of significance in the study of the related fields.

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