Inconsistency between height-height correlation and power-spectrum functions of scale-invariant surfaces for roughness exponent $\alpha \sim 1$

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The height-height correlation function $H(\mathbf{r})$ from a scale-invariant surface is compared with the corresponding power-spectrum function $W(\mathbf{q})$ using a variety of mathematical scaling functions. We show that for a non-self-affine surface with the roughness exponent $\alpha \ge 1$, one of the asymptotic scaling relations, either $H(\mathbf{r}) \sim r^{2\alpha}$ or $W(\mathbf{q}) \sim q^{-2\alpha-d}$, can be violated. An inconsistency in the values of α also exists between $H(\mathbf{r})$ and $W(\mathbf{q})$ when $\alpha > 0.9$. The impact on the data analysis using different experimental methods is discussed.

I. INTRODUCTION

Many physical processes, such as fracture, erosion, etching, and thin-film growth, can produce rough-surface morphologies, which exhibit scale-invariant behaviors. A rough surface having scaling characteristics can be described by a height-height correlation function, 1,2

$$H(\mathbf{r}) = \langle [h(\mathbf{r}) - h(0)]^2 \rangle = 2w^2 f(r/\xi)$$

$$= \begin{cases} (r/\eta)^{2\alpha} & \text{for } r << \xi \\ 2w^2 & \text{for } r >> \xi \end{cases}, \tag{1}$$

where $h(\mathbf{r})$ is the surface height at the horizontal position $\underline{\mathbf{r}}$. \underline{w} represents the interface width, $w = \sqrt{\langle [h(\mathbf{r}) - \langle h \rangle]^2 \rangle}$, which is a measure of the vertical amplitude of fluctuation in rough surfaces. ξ is the lateral correlation, a distance within which the surface-height fluctuations are correlated but beyond which the variations spread and are not correlated. $\eta^{-1} = w^{1/\alpha}/\xi$ describes the average local slope of the surface. The scaling function f(x) has an asymptotic form,

$$f(x) = \begin{cases} x^{2\alpha} & \text{for } x \ll 1\\ 1 & \text{for } x \gg 1 \end{cases}$$
 (2)

The scaling behavior manifests itself in a power-law form, $H(\mathbf{r}) \sim r^{2\alpha}$, which exists on the short-range scale $r \ll \xi$. The exponent α describes surface roughness. For most scale-invariant surfaces, α is limited within the range $0 \le \alpha < 1$, where the morphology is a self-affine fractal with an "anisotropic" scaling relationship between vertical and lateral directions. Recently, there are indications that a non-self-affine scaling can exist in either an etched surface⁴ or thin films produced by molecular-beam-epitaxy (MBE) processes, $^{5-7}$ where α can be equal to 1, as is consistent with recent theoretical predictions. $^{8-13}$

Experimentally, there are three methods to measure the roughness exponent α . First, one can obtain α by using real-space image techniques to directly measure the height-height correlation function or the finite-size interface width. Examples were those using the ball stylus, ¹⁴

scanning tunneling microscopy (STM), $^{15-20}$ and atomic-force-microscopy 21,22 (AFM) techniques. The second method employs diffraction techniques to measure either the diffuse diffraction intensity $I_{\rm diff}$ or the full width at half-maximum (FWHM) of the diffuse diffraction line shape, as a function of the perpendicular diffraction momentum transfer k_1 . The measurements are based on the rigorous power-law relationships, $^{23-25}$ $I_{\rm diff} \sim k_1^{-2/\alpha}$ and FWHM $\sim k_1^{1/\alpha}$, as a result of the diffraction from a scaling surface described by Eq. (1). Such an indirect method is valid for the diffraction condition $k_1 w > 1$, which is suitable for the high-resolution low-energy electron-diffraction (HRLEED), 4,7,26 x-ray, 20,27 and He scattering techniques. Recently, by modifying the measurement geometry, we have been able to apply the analysis in an angle-resolved-light-scattering (ARLS) experiment. In the third method, one determines α by measuring the power-spectrum function,

$$W(\mathbf{q}) = |h_{\mathbf{q}}|^2 \,, \tag{3}$$

where h_q is the Fourier transform of the surface height, $h_q = \int d\mathbf{r} \, h(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}}$. For a self-affine surface characterized by Eq. (1), the corresponding power spectrum has a power-law tail shape, ^{28,29}

$$W(\mathbf{q}) \sim q^{-2\alpha - d}$$
 as $q \gg \xi^{-1}$, (4)

where d (=1 or 2) denotes the dimensionality. Equation (4) can be measured from diffraction techniques under the diffraction condition $k_{\perp}w \ll 1$. At such a small k_{\perp} condition, the diffuse intensity is a measure of the power-spectrum function, $I_{\rm diff}(\mathbf{k}_{\parallel}) \sim W(\mathbf{k}_{\parallel})$, where $\mathbf{k}_{\parallel}(=\mathbf{q})$ is the diffraction momentum transfer parallel to the surface. Practically, in real-space image techniques, one often utilizes the power-spectrum method to determine α in order to have better statistics, 17,19 where the digitized surface height $h(\mathbf{r})$ from a measured image surface is Fourier transformed to $h_{\mathbf{q}}$ in order to calculate the power-spectrum function, Eq. (3). Although the three methods mentioned above are different, it was expected that the results should be consistent with each other within experimental accuracy.

In a previous study,³⁰ the validity of the diffraction method was examined using several mathematically acceptable functions for the height-height correlation function. The comparison between a STM result and x-ray-reflectivity data confirmed the consistency between the first method using real-space image techniques and the second method using diffraction techniques. However, so far, the consistency between the power-spectrum method and the first two methods has not been examined.

In this paper, we give a detailed comparison between the height-height correlation and the corresponding power-spectrum function using a variety of mathematical scaling functions. We show that the results can be inconsistent when $\alpha > 0.9$. Such a difference becomes more dramatic for a non-self-affine surface $\alpha \ge 1$, where one of the scaling relations, either $H(\mathbf{r}) \sim r^{2\alpha}$ or $W(\mathbf{q}) \sim q^{-2\alpha-d}$, can be violated. The impact of different methods on the data analysis will be discussed.

II. GENERAL RELATIONSHIP BETWEEN HEIGHT-HEIGHT CORRELATION FUNCTION AND POWER-SPECTRUM FUNCTION

The connection between $H(\mathbf{r})$ and $W(\mathbf{q})$ can be obtained through the autocovariance height correlation function,

$$\langle h(\mathbf{r})h(0)\rangle = \frac{1}{2} \{\langle [h(\mathbf{r})]^2 \rangle + \langle (h(0))^2 \rangle - \langle [h(\mathbf{r}) - h(0)]^2 \rangle \}$$

$$= w^2 - \frac{1}{2} H(\mathbf{r}) = w^2 [1 - f(r/\xi)], \qquad (5)$$

where the last step is obtained using Eq. (1). Given a height-height correlation function shown as Eq. (1), one can calculate the power-spectrum function as

$$W(\mathbf{q}) = |h_{\mathbf{q}}|^{2} \sim \int d\mathbf{r} \, e^{i\mathbf{q}\cdot\mathbf{r}} \langle h(\mathbf{r})h(0) \rangle$$

$$\sim \int d\mathbf{r} \, e^{i\mathbf{q}\cdot\mathbf{r}} [1 - f(r/\xi)]$$

$$\sim g(q\xi) = g(Q) , \qquad (6)$$

where $Q = q\xi$ and g(Q) is the reciprocal-space scaling function. Corresponding to the real-space scaling function given by Eq. (2), g(Q) could be expected to behave as

$$g(Q) \sim \begin{cases} 1 & \text{for } Q \ll 1 \\ Q^{-2\alpha - d} & \text{for } Q \gg 1 \end{cases}, \tag{7}$$

which is consistent with Eq. (4). The validity of the relationship between Eqs. (2) and (7) shall be examined later.

On the other hand, if the power-spectrum function is known, one can obtain the height-height correlation function,

$$H(\mathbf{r}) = 2w^{2} - 2\langle h(\mathbf{r})h(0)\rangle$$

$$\sim \int d\mathbf{q}(1 - e^{-i\mathbf{q}\cdot\mathbf{r}})W(\mathbf{q}), \qquad (8)$$

where based on Eq. (6), we have $\langle h(\mathbf{r})h(0)\rangle = \int d\mathbf{q} e^{-i\mathbf{q}\cdot\mathbf{r}}W(\mathbf{q})$ and $w^2 = \langle [h(0)]^2\rangle = \int d\mathbf{q}W(\mathbf{q})$. Using Eqs. (6) and (8) in the next section, we shall examine the relationships between $H(\mathbf{r})$ and $W(\mathbf{q})$ [f(x) and g(Q)] for a variety of given scaling form functions.

III. COMPARISON OF THE SCALING RELATIONSHIP BETWEEN HEIGHT-HEIGHT CORRELATION AND POWER-SPECTRUM FUNCTIONS

In the following discussion, we focus on four model scaling functions that are not only mathematically acceptable but also analytically solvable. In model 1 and model 2, we start from given real-space scaling functions and then calculate the corresponding reciprocal-space scaling functions, i.e., $f(x) \Longrightarrow g(Q)$, based on Eq. (6). In contrast, in model 3 and model 4, we derive the real-space scaling functions from given reciprocal-space scaling functions, i.e., $g(Q) \Longrightarrow f(x)$, according to Eq. (8).

A. Model 1: The real-space scaling function: $f(x) = 1 - e^{-x^{2\alpha}}$

This phenomenological scaling function was proposed by Sinha et al.²⁴ At short distance, x << 1, the function $f(x)=1-e^{-x^{2\alpha}}$ behaves as a power law, $x^{2\alpha}$. But at large distance, x >> 1, it approaches 1 exponentially, which is consistent with many physical systems. Substituting this real-space scaling function into Eq. (6), we obtain the corresponding power-spectrum function, $W(\mathbf{q}) \sim \int d\mathbf{r} \, e^{i\mathbf{q}\cdot\mathbf{r}} e^{-(r/\xi)^{2\alpha}}$. The analytical solution can be obtained in two cases: $\alpha=0.5$ and $\alpha=1$. For $\alpha=0.5$, one has

$$W(\mathbf{q}) = \frac{1}{[1 + (q\xi)^2]^{(1+d)/2}} \sim q^{-1-d} \text{ as } q \gg \xi^{-1}$$
,

which is consistent with the scaling relation, $\sim q^{-2\alpha-d}$. However, for $\alpha=1$, we have

$$W(\mathbf{q}) = e^{-(1/4)(q\xi)^2}$$
,

which decays exponentially when $q \gg \xi^{-1}$ (or $Q = q \xi \gg 1$) and does not agree with the power-law decay, $\sim q^{-2\alpha - d}$, as shown in Eqs. (4) and (7).

B. Model 2: The real-space scaling function: $f(x) = 1 - e^{-x^2} (1 - Cx^{2\alpha})$

Within the range $0 < \alpha \le 1$, the function $1 - e^{-x^2}(1 - Cx^{2\alpha})$ satisfies the scaling condition given by Eq. (2), where C is a constant 0 < C < 1. Similar to model 1, this function approaches 1 exponentially as $x \to \infty$, and therefore it is physically acceptable. The advantage for this function is that the corresponding power-spectrum function is analytically solvable for any values of α , as given by 3^{1}

$$W(\mathbf{q}) \sim e^{-(1/4)(q/\xi)^2} - C'M\left[\alpha + \frac{d}{2}, \frac{d}{2}, -\frac{(q\xi)^2}{4}\right],$$
 (9)

where $C' = C\Gamma(\alpha + d/2)/\Gamma(d/2)$ and $\Gamma(x)$ is the gamma function. $M(\alpha + d/2, d/2, -(q\xi)^2/4)$ is the Kummer function defined as³¹

$$M(a,b,z) = \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b)}{\Gamma(b+n)\Gamma(a)} \frac{z^n}{n!}.$$

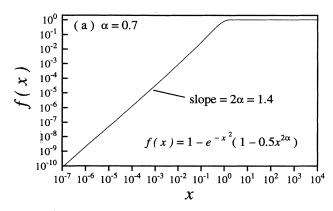
Asymptotically, as $q \gg \xi^{-1}$, Eq. (9) can be simplified as

$$W(\mathbf{q}) \sim \begin{cases} q^{-2\alpha-d} & \text{for } \alpha \neq m \\ e^{-(1/4)(q\xi)^2} & \text{for } \alpha = m \end{cases}$$

where m is a positive integer. Obviously, only when $\alpha \neq m$ can this power-spectrum function agree with the scaling relation, $\sim q^{-2\alpha-d}$. To demonstrate these scaling relations, we plot the real-space scaling function, $f(x)=1-e^{-x^2}(1-Cx^{2\alpha})$ for $\alpha=0.7$, and the corresponding power-spectrum function, Eq. (9), in log-log scale shown in Figs. 1(a) and 1(b), respectively. From the slope shown in each figure, one can obtain the value of α . It is shown that the values of α obtained from f(x) and W(q) are consistent with each other for this self-affine surface.

C. Model 3: The reciprocal-space scaling function: $g(Q) = (1 - e^{-Q^{2\alpha+d}})/Q^{2\alpha+d}$

In contrast to model 1 and model 2, which are phenomenological functions, the reciprocal scaling function $(1-e^{-Q^{2\alpha+d}})/Q^{2\alpha+d}$ can be originated from the thin-film growth dynamics. For example, when $2\alpha+d=2$, it cor-



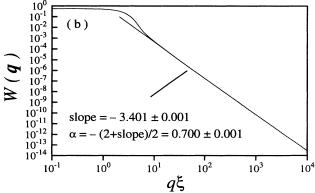


FIG. 1. Log-log plot for (a) the real-space scaling function $f(x)=1-e^{-x^2}(1-Cx^{2\alpha})$ for $\alpha=0.7$; and (b) the corresponding power-spectrum function. From the slope shown in each figure, one can extract the value of α .

responds to a model of random growth with diffusion. ³² For $2\alpha+d=4$, it corresponds to a MBE growth model with linear diffusion dynamics. ⁸⁻¹³ In these two cases, the corresponding height-height correlations can be calculated analytically. The asymptotic forms for $r \ll \xi$ are shown as follows.

(i) Random-growth model with diffusion $(2\alpha + d = 2)$:

$$H(\mathbf{r}) \sim \begin{cases} r & \text{for } d = 1 \text{ and } \alpha = 0.5\\ \ln(r) & \text{for } d = 2 \text{ and } \alpha = 0 \end{cases}, \tag{10}$$

which is consistent with the general scaling form, $H(\mathbf{r}) \sim r^{2\alpha}$.

(ii) MBE growth model $(2\alpha + d = 4)$:¹³

$$H(\mathbf{r}) \sim \begin{cases} r^2 & \text{for } d = 1 \text{ and } \alpha = 1.5 \\ r^2 \ln(\xi/r) & \text{for } d = 2 \text{ and } \alpha = 1. \end{cases}$$
 (11)

Similar to the cases for $\alpha = 1$ shown in models 1 and 2, the height-height correlation for $\alpha \ge 1$, shown as Eq. (11), violates the general scaling form, $H(\mathbf{r}) \sim r^{2\alpha}$.

D. Model 4: The reciprocal-space scaling function: $g(Q) = 1/(1+Q^2)^{\alpha+d/2}$

This Lorentzian type of scaling function is perhaps the most simple and acceptable form that satisfies Eq. (7). The Lorentzian line shapes are commonly observed in diffraction experiments. Besides, one of the advantages for this function is that for any values of α , the corresponding height-height correlation function is analytically solvable:³¹

$$H(\mathbf{r}) \sim B - (r/\xi)^{\alpha} K_{\alpha}(r/\xi) , \qquad (12)$$

where B is a constant, $B = x^{\alpha}K_{\alpha}(x)|_{x=0}$, and $K_{\alpha}(r/\xi)$ is the modified Bessel function, which vanishes exponentially as $r \gg \xi$ or $x = r/\xi \gg 1$. We are more interested in the asymptotic form of Eq. (12) on the short range of $r \ll \xi$, which can be simplified as³¹

$$H(\mathbf{r}) \sim \begin{cases} r^{2\alpha} - O(r^2) & \text{for } 0 < \alpha < 1 \\ r^2 \ln(\xi/r) & \text{for } \alpha = 1 \\ r^2 - O(r^{2\alpha}) & \text{for } 1 < \alpha < 2 \end{cases},$$
 (13)

where O() denotes the higher-order term. It is shown again that when $\alpha \ge 1$, the scaling function violates the general scaling form $H(\mathbf{r}) \sim r^{2\alpha}$. Note that for $\alpha = 1$, Eqs. (11) and (13) are quite similar although they are derived from different power-spectrum functions. To demonstrate the scaling behavior, in Figs. 2(a) and 2(b), we plot in log-log scale the Lorentzian type of reciprocal-space scaling function, $g(Q)=1/(1+Q^2)^{\alpha+d/2}$, for $\alpha=1.0$, and the corresponding height-height correlation function, Eq. (12), respectively. From the slope shown in each figure, we can obtain the value of α , where the slopes are extracted at the ranges, $10^2 \le Q \le 10^4$, in Fig. 2(a) and $10^{-7} \le r/\xi \le 10^{-4}$ in Fig. 2(b), respectively. Figure 3 shows a comparison of the extracted α from g(Q) (dashed curve) and that from Eq. (12) (solid curve). It is shown that the deviation between the extracted values α

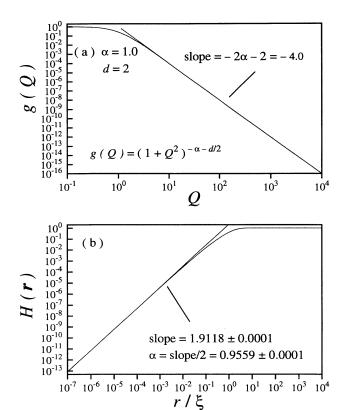


FIG. 2. Log-log plot of (a) the Lorentzian type of power-spectrum scaling function, $g(Q)=1/(1+Q^2)^{\alpha+d/2}$, for $\alpha=1.0$; and (b) the corresponding height-height correlation function.

obtained from the power-spectrum function and the height-height correlation function occurs when $\alpha > 0.9$.

IV. DISCUSSION

We learned from the preceding section that if the roughness exponent $\alpha \ge 1$, one of the scaling relations, either $H(\mathbf{r}) \sim r^{2\alpha}$ or $W(\mathbf{q}) \sim q^{-2\alpha-d}$, must be violated, which is a characteristic of non-self-affine surfaces. Such a violation leads to an inconsistency in the result of data analysis between the power-spectrum method and the other two methods mentioned in the Sec. I. The impact on the experimental analysis can be significant.

For example, if the roughness exponent is found to be $\alpha=1$ using the power-spectrum method, the surface can be concluded to have a non-self-affine morphology. However, as shown in Figs. 2(b) and 3, the measurement from the same surface using a diffraction technique (or an imaging technique) can give a value of $\alpha \approx 0.96$, which may lead to a conclusion of a self-affine surface. Such a discrepancy in the values of α was also noticed by Amar and co-workers¹³ when they tried to determine α from Eq. (11). Note that the value of α is obtained from a short range between $r = 10^{-7}\xi$ and $r = 10^{-3}\xi$, which is accurate enough to show the asymptotic power-law relation. Such an ideal short range may not be easily realized for a practical system. For example, one needs a technique to be able to scan at least a range of $10^7 \text{ Å} = 1000$

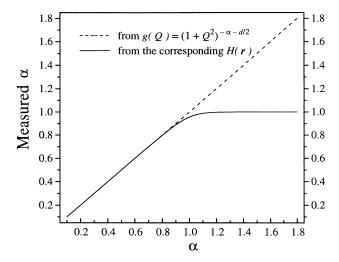


FIG. 3. Comparison between the values of α extracted from the Lorentzian type of power-spectrum function (dashed curve) and from the corresponding height-height correlation function (solid curve). The deviation between the two curves occurs when $\alpha > 0.9$.

 μ m with ~1-Å spatial resolution while the surface has a lateral correlation length ξ ~1000 μ m. If a more realistic measure of the short range is chosen, such as from $r=10^{-4}\xi$ and $r=10^{-1}\xi$, one will obtain $\alpha\approx0.91$, which deviates even more from $\alpha=1$.

We must emphasize that the inconsistency between the values of α from different methods not only exists when $\alpha \ge 1$, but also occurs in self-affine surfaces with α in the region $0.9 < \alpha < 1$, as shown in Fig. 3. The origin for this discrepancy can be understood from Eq. (13). As α is closer to 1 from below, the magnitude of the leading term $r^{2\alpha}$ will become comparable to that of the higher-order term O(2) and therefore the determination of α must be affected by the higher-order contributions.

In conclusion, an inconsistency in the values of α exists between the height-height correlation function and the power-spectrum function obtained from the same surface when $\alpha > 0.9$. For a non-self-affine surface where $\alpha \ge 1$, one of the scaling relations, either $H(\mathbf{r}) \sim r^{2\alpha}$ or $W(\mathbf{q}) \sim q^{-2\alpha-d}$, can be violated. The implication of this inconsistency is that one must understand the relationship between the results obtained by the power-spectrum analysis and by the real space or diffraction methods for $\alpha > 0.9$. Besides, when $0.9 < \alpha < 1$, we should be aware of the sensitivity and the accuracy of α to the chosen measurement range where the slopes of the height-height correlation function are determined using either realspace image techniques or diffraction techniques. In other words, one should be cautious when analyzing the experimental data obtained from a scaling surface with α close to 1.

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