Self-affine fractals and the limit $H \to 0$

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A modified form for the surface-height-fluctuation correlation function of rough surfaces, $g_\gamma(R) \propto \int_{a_0/\xi}^{R/\xi} x^{2H}(e^{-x}/x)dx$, is investigated which depicts behavior related to self-affine fractals for $0<H<1$, and for $H \to 0$ with $a_0 \ll R \ll \xi$ reveals logarithmic behavior $g_\gamma(R) \propto \ln(R/a_0)$.

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Recently, there has been considerable interest in the study of stochastically growing surfaces in the context of various surface growth models from theoretical and experimental points of view [1]. In general, nonequilibrium effects introduce a relevant nonlinearity which causes an anomalous power-law growth of the height fluctuations [2]. Under certain conditions this power law can be replaced by a logarithmic law [3–6]. In the latter case the short-range roughness exponent H is equal to zero, which is a rather subtle situation since a three-dimensional object can be either a fractal or a Euclidean volume. In the context of surface-roughness studies, the knowledge of the surface height correlation function is essential not only for the determination of characteristic surface parameters, but also for an understanding of the impact of the surface morphology on various physical phenomena.

The type of rough surface in the static phase we shall consider here is the so-called solid-on-solid model, in which the surface is defined by a vertical height profile above a horizontal xy plane, and is represented by a single-valued random function $z(\mathbf{r})$ of the in-plane positional vector $\mathbf{r}=(x,y)$. The difference $z(\mathbf{r})-z(\mathbf{r}')$ is assumed to be a Gaussian random variable whose distribution depends on the relative coordinates $(x'-x,y'-y)$ such that $g(\mathbf{R})=\langle[z(\mathbf{r})-z(\mathbf{r}')]^2\rangle$, $\mathbf{R}=\mathbf{r}'-\mathbf{r}$. For an isotropic surface in x-y directions we may assume that

$$g(\mathbf{R}) = AR^{2H}, \tag{1}$$

with $0<H<1$. This kind of surface roughness can be attributed to self-affine fractal surfaces as defined by Mandelbrot in terms of fractional Brownian motion [7]. The roughness exponent H determines the surface texture, and is associated with a local fractal dimension $D=3-H$ [7,8]. For $R \to \infty$, $g(R) \to \infty$ and $g(R)/R^2 \to 0$ (surface asymptotically flat), which is a rather ideal case since on real surfaces $g(R)$ at large length scales may saturate to the value $2\sigma^2$. The parameter $\sigma=\langle z(\mathbf{0})^2\rangle^{1/2}$ is the rms-saturated surface roughness. This implies the existence of an effective roughness cutoff ξ (correlation length) such that for $R \ll \xi$, $g(R) \propto R^{2H}$ [9,10]. Therefore, on real surfaces $g(R)$ satisfies the following conditions:

$$g(R) \propto R^{2H}, \quad R \ll \xi, \tag{2a}$$

$$g(R) = 2\sigma^2, \quad R \gg \xi, \tag{2b}$$

with $0<H<1$.

Up to now the functional form for $g(R)$ which has been used in the literature to incorporate finite-size effects for self-affine fractals in the static phase has the form $g(R)=2\sigma^2[1-e^{-(R/\xi)^{2H}}]$ [9,10]. The exponential term in the previous equation is the well-known Kohlrausch-Williams-Watts function which has been used to fit miscellaneous experimental data [8–11]. However, this function does not address the $H=0$ case, which is related to the existence of a lower fractal bound, and is of fundamental interest to account for predictions related to the nonequilibrium roughening transition [3–6]. Rather, it reveals a trivial behavior. Wong *et al.* [12] have introduced a scaling form for $g(R)$ when $H=0$, in order to incorporate finite-size effects (finite ξ) in scattering studies of logarithmic roughness related to the roughening transition, which, however, does not arise as a limiting case of self-affine fractal correlation of finite ξ.

Therefore, our purpose in this paper is to investigate an alternative functional form for $g(R)$ which for $0<H<1$ reveals characteristics related to self-affine fractals, and in the limit $H \to 0$ possesses a nontrivial (logarithmic) behavior. The proposed form for $g(R)$ is the following:

$$g_\gamma(R) = 2\sigma^2 B_\gamma(H) \int_{a_0/\xi}^{R/\xi} x^{2H} \frac{e^{-x}}{x} dx, \tag{3a}$$

$$B_\gamma(H) = \left[\int_{a_0/\xi}^{L_m/\xi} x^{2H} \frac{e^{-x}}{x} dx \right]^{-1}, \tag{3b}$$

where a_0 is the atomic spacing, and L_m the macroscopic surface size.

The choice of this particular form to describe $g(R)$ has its origin in critical phenomena, as well as in previous studies of fractal systems. In fact, Eqs. (3) have been introduced in a manner analogous to that used in critical phenomena [13], and in x-ray scattering studies of fractal aggregates where, apart from the integration over the length scales (a_0,R), the corresponding expression of the pair correlation function has the form $\sim R^{D-3}e^{-R/\xi}$ with D being the fractal dimension [14].

The small-length-scale behavior of Eq. (3a) has the following characteristics. For $a_0 \ll R \ll \xi$,

$$g_\gamma(R) \approx [2\sigma^2] \frac{B_\gamma(H)}{2H} [(R/\xi)^{2H} - (\xi/a_0)^{2H}] \propto R^{2H}, \tag{4}$$

which is consistent with the self-affine nature for $0<H<1$. In addition, in the limit $H\rightarrow 0$,

$$g_\gamma(R)|_{H\rightarrow 0}\approx 2\sigma^2 B_\gamma(0)\ln(R/a_0)\ . \tag{5}$$

This logarithmic behavior is met in the context of various surface growth models related to the roughening transition [3–6]. In general, for purely two-dimensional systems, if we ignore finite-size effects, the capillary wave fluctuations cause $g(R)$ to follow a logarithmic behavior, $g(R)\sim\ln(R)$ [9]. Equations (4) and (5) imply that the small-length-scale expansion of self-affine fractal surfaces has to be in general of the form

$$g(R)\approx\frac{A}{2H}[(R/a_0)^{2H}-1] \tag{6}$$

in order to be consistent with the characterization that the surface becomes more irregular as H becomes smaller. Specifically, $g_\gamma(R)/\sigma^2$, which represents a measure of the height-height-fluctuation density, acquires larger values as H decreases, resulting in more dense surface height-height fluctuations or more jagged surfaces (Fig. 1). Such behavior is related to the existence of a lower fractal bound, which is necessary in order that the logarithmic behavior arises from power-law fluctuations [12,15].

We illustrate in general the applicability of Eqs. (3) (which can be relevant in experimental studies [9,10,12]) in terms of a fit to correlation data acquired from a 100.0-nm-thick silver film, thermally evaporated on a polished quartz crystal held at 106 K. The system base pressure was $\sim 5\times 10^{-8}$ Torr, and $\sim 5\times 10^{-7}$ Torr during deposition. The silver film was left to be annealed until it reached room temperature. The correlation data acquired by means of scanning tunneling microscopy (STM) in a dry N_2 gas environment. The scan size was 500.0 nm with 400 points per line scan, and four files of correlation data acquired at different locations on the surface have been averaged. The value of H in terms of a power-law fit is $H_p=0.72\pm 0.05$ (inset). A fit of Eqs. (3) has been performed with $H_\gamma=0.69$ $L_m=10^6$ nm, and $a_0=0.27$ nm (solid line). During the fit parameters a_0 and L_m were kept constant to the previous values, which were used as a typical atomic spacing for silver atoms, and macroscopic sample size. Essentially, since $L_m\gg\xi$ the fit is insensitive to the particular choice of the microscopic surface size, where the ratio L_m/ξ can be considered to be infinite. The value of $\sigma\approx 1.0$ nm has been estimated for every image directly using the STM utility to calculate the rms surface roughness over a surface area 500×500 nm^2, and averaged over the four data files (ensemble average). In this manner, $2\sigma^2$ essentially corresponds to the large-distance value of $g(R)$, $R\gg\xi$, over the scan size used to acquire the correlation data (~ 500.0 nm). However, since σ^2 represents a normalization factor, it has been removed from the data during the fit in order to focus mainly on the two surface parameters H and ξ. The parameters H and ξ were varied during the fit in a restrictive manner, as is explained below. The parameter H_γ was allowed to deviate from the power-law fit values $H_p=0.72$ only by ± 0.05 in order for the fit to have physical meaning, since the power-law fit determines uniquely the roughness exponent H to within the specified limit of accuracy. The correlation length ξ can be determined as the length scale for which $g(R)$ acquires the value $g(\xi)$. However, in order for the correlation length and subsequently $g(R)$ to have real significance, ξ has to be located in the regime where a remarkable deviation from power-law behavior occurs. In our case this occurs for $g(R=\xi)\approx 1$, and the corresponding length scale from the data [squares, Fig. 1] yield $\xi_\gamma=9.5\pm 0.5$ nm. ξ_γ was allowed to vary during the fit from the value 9.5 nm only in between the specificed limits of accuracy, ± 0.5. The value of ξ_γ is of real significance for the corresponding surface morphology, since it is located in the regime where a remarkable deviation occurs from linear (power-law) behavior, and also compares favorably with cluster sizes obtained from STM images.

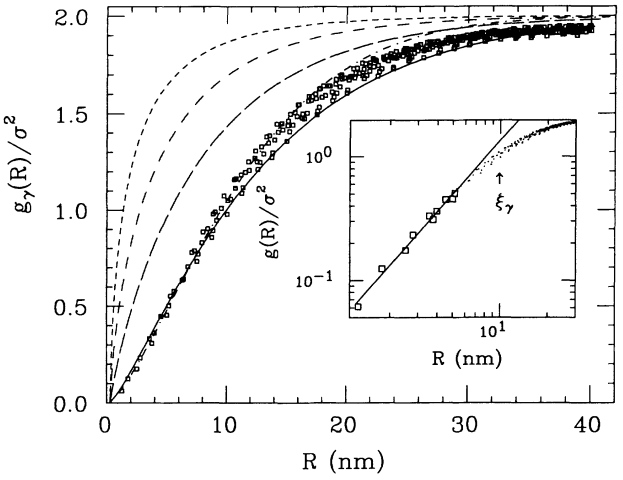

FIG. 1. Schematics for $g_\gamma(R)/\sigma^2$ as a function of H, $\xi=9.3$ nm, $a_0=0.27$ nm. $H=0.0$: small dashes; $H=0.2$: dashes; $H=0.4$: long dashes. The solid line depicts a fit of Eqs. (3) to the correlation data (squares) of the annealed 106-K silver film, with $H_\gamma=0.69$, and $\xi_\gamma=9.3$ nm, as well as $a_0=0.27$ nm and $L_m=10^6$ nm. The fit to the function $g(R)/\sigma^2=2[1-e^{-(R/\xi)^{2H}}]$ is shown, with $H=0.72$ and $\xi=12.3$ nm (dot-dashed line). The inset depicts a power-law fit (squares) to determine H, which gives $H_p=0.72\pm 0.05$. The arrow indicates the position of the correlation length ξ_γ with respect to the regime where significant deviation from power-law behavior occurs.

In conclusion, the aim of this paper was to introduce a modified scaling form of the surface-height-fluctuation correlation function $g(R)$, which in the limit $H\rightarrow 0$ posses logarithmic behavior. Direct comparison with correlation data shows the adequacy of this form to describe real surface correlations beyond the power-law regime. At the same time the traditional fit using the Kolrausch-Williams-Watts function $g(R)/\sigma^2=2[1-e^{-(R/\xi)^{2H}}]$ for the same data (Fig. 1) is significantly good in the regime of length scales $R\leq 2\xi$ with $\xi=12.3$ nm [determined from the length scale that corresponds to $g(R=\xi)/\sigma^2$]. Furthermore, Eqs. (2) can be relevant in a larger scale of experimental studies, e.g.,

where information for the surface morphology is obtained though $g(R)$, and especially for the cases in which the roughness exponent H attains significantly small values or becomes zero [9,10,12].

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[1] *Dynamics of Fractal Surfaces,* edited by F. Family and T. Viscek (World Scientific Singapore, 1991).

[2] M. Kardar, G. Parisi, and Y. Zhang, Phys. Rev. Lett. **56**, 889 (1986).

[3] J. G. Amar and F. Family, Phys. Rev. Lett. **64**, 543 (1990).

[4] J. Krug *et al.,* Phys. Rev. Lett. **64**, 2332 (1990); J. M. Kim *et al., ibid.* **64**, 2333 (1990); D. A. Huse *et al.,* Phys. Rev. A **41**, 7075 (1990).

[5] T. Hwa, M. Kardar, and M. Paczuski, Phys. Rev. Lett. **66**, 441 (1990).

[6] B. M. Forrest and L. Tang, Phys. Rev. Lett. **64**, 1405 (1990).

[7] B. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, New York, 1982).

[8] S. Alexander, in *Transport and Relaxation in Random Materials,* edited by J. Klafter, R. Rubin, and M. F. Schlesinger (World Scientific, Singapore, 1987).

[9] S. K. Sinha, E. B. Sirota, S. Garoff, and H. B. Stanley, Phys. Rev. B **38**, 2297 (1988).

[10] R. Pynn, Phys. Rev. B **45**, 602 (1992); W. Weber *et al., ibid.* **46**, 7953 (1992); G. Palasantzas *et al., ibid.* **48**, 2873 (1993).

[11] G. Williams and D. C. Watts, Trans. Faraday Soc. **66**, 80 (1970); *Non-Debye Relaxation in Condensed Matter,* edited by T. V. Ramarkrishnan and M. Raj Lakshmi (World Scientific, Singapore, 1987); *Polymer Motion in Dense Systems,* edited by D. Richter and T. Springer (Springer-Verlag, Berlin, 1988).

[12] P. Z. Wong *et al.,* Phys. Rev. B **37**, 7751 (1988); J. Appl. Cryst. **21**, 786 (1988).

[13] P. A. Egelstaff, *An Introduction to the Liquid State* (Academic, London, 1967), p. 211.

[14] *On Growth and Form,* edited by H. E. Stanley and N. Ostrowsky (Martinus Nijhoff, Boston, 1986).

[15] The logarithmic roughness follows from the power-law roughness in the limit $H \rightarrow 0$, if we consider the limiting form $\lim_{H \rightarrow 0}(1/H)[x^H - 1] \rightarrow \ln(x)$.