

Roughness exponents: A paradox resolved

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The spatial scaling behavior of a self-affine surface is parametrized with what is commonly referred to as a “roughness” exponent. The paradox of whether large or small values of this exponent correspond to “rougher” surfaces is resolved here.

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A wide variety of surfaces and interfaces occurring in nature are well represented by a kind of roughness associated with self-affine fractal scaling, defined by Mandelbrot in terms of fractional Brownian motion [1]. Examples include the nanometer scale topology of vapor-deposited films [2], the spatial fluctuations of liquid-gas interfaces [3], and the kilometer scale structures of mountain terrain [1]. Physical processes which produce such surfaces are wide ranging. They include fracture [4], erosion [5], and molecular-beam epitaxy [6], as well as fluid invasion of porous media [7]. Self-affine surfaces are characterized by fluctuations perpendicular to the surface whose width σ is defined as the height fluctuation over a length scale L parallel to the surface,

$$\sigma(L, t) = \langle [h(r, t) - \langle h(r, t) \rangle]^2 \rangle^{1/2}, \quad (1)$$

where t denotes time, h the height, and $\langle \rangle$ the spatial average over position r in a planar reference surface. This width scales with L and t as [8]

$$\sigma(L, t) = L^\alpha f(tL^{-\alpha/\beta}). \quad (2)$$

We focus here on the “static” roughness, which is achieved at times t much larger than a saturation time $t_{\text{sat}} \propto L^{\alpha/\beta}$, so that [9]

$$\sigma \propto L^\alpha. \quad (3)$$

The exponent α normally ranges between 0 and 1 and is generally referred to as the “roughness exponent.” Also denoted by H , χ , ζ , and h , it has variously been referred to in the literature as the “Hurst,” or “Holder” exponent, the “static roughness” parameter, and the “stationary,” or “spatial” scaling parameter.

In a recent publication involving numerical simulation of nonequilibrium film growth, Yan found it surprising that specific inclusion of surface diffusion effects in simulation could result in an increase in the roughness parameter [10]. The implication is that surface diffusion should *smooth* the surface, while an increased roughness exponent is indicative of a *rougher* surface. Yan has good reason to be puzzled: numerous authors [11] explicitly state in their respective publications that large values of α correspond to rough surfaces. Other authors [12], following the mathematical definitions of Mandelbrot, assert that large values of α correspond to surfaces with a “smooth texture.” Clearly there is a paradox, if not a

contradiction. These two schools of thought have remained virtually nonoverlapping, even though they employ the identical formalism to define the roughness exponent. Our purpose here is to reconcile the two points of view, and to clarify the paradox.

Consider Fig. 1, taken from Ref. [2]. Three surface profiles are presented, with roughness exponents (termed H in Ref. [2]) ranging from 0.3 to 0.7. The profile with the largest roughness exponent has the “smoothest” texture. We note that all three profiles have the same width on the scale of the sample size, $\sigma_{\text{max}} \equiv \sigma(L_{\text{max}}) \approx 1.1$. Here, as in much of solid-state physics and fractal phenomena, the roughness exponent is defined within the context of a *microscopic limit*, $L \rightarrow 0$, which describes how σ varies from the linear sample size L_{max} down to atomic length scales. The limit is usually taken under the assumption of a fixed surface width σ_{max} on the scale of L_{max} . Thus the limit $\alpha = 0$ corresponds to a *very jagged* (and therefore very rough) surface, characterized by a nearly constant width σ down to microscopic parallel length scales L . For $\alpha > 0$, a smoother surface results, since σ decreases with decreasing L . Within this context,

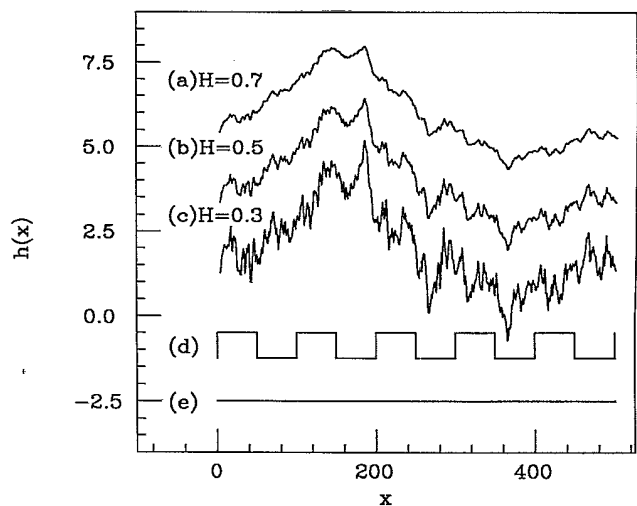


FIG. 1. Figure 1 of Ref. [2] (Chiarello *et al.*). Profiles (a), (b), and (c) are self-affine with roughness exponents α (termed H in that publication) ranging from 0.3 to 0.7. The self-affine profiles all have the same rms width $\sigma = 1.1 \pm 0.1$.

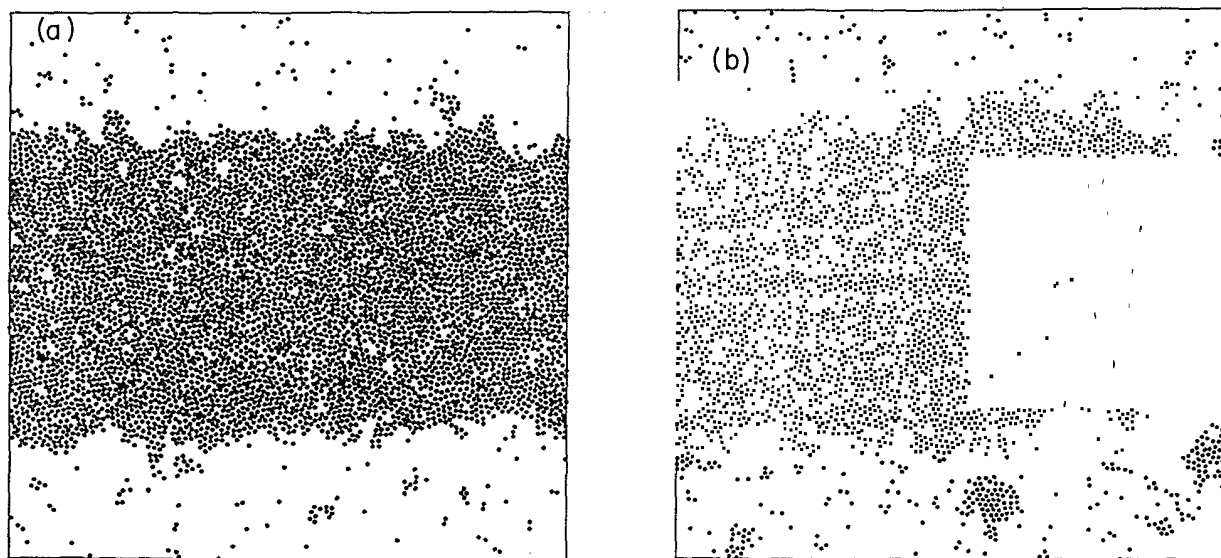


FIG. 2. A snapshot of liquid-vapor interfaces in a molecular-dynamics simulation of a two-dimensional Lennard-Jones fluid. These interfaces are characterized by $\alpha=0$ in the presence of an external gravitational field [Fig. 2(a)], and by $\alpha=1/2$ in zero gravity [Fig. 2(b)]. (Reprinted with permission from the first and second sources in Ref. [3].)

larger values of α correspond to smoother surfaces. The effect of surface diffusion is to *increase* α , or *smooth* a surface, since local rearrangement of atoms will have a greater impact on the shorter parallel length scales.

In contrast, in the field of statistical mechanics, α is defined in the *thermodynamic limit*, $L \rightarrow \infty$, and describes an asymptotic property of an interface at large length scales. The interfacial width, for example that of the two liquid-vapor interfaces depicted in Fig. 2, is fixed at small length scales by the (microscopically small) bulk correlation length ξ . On length scales larger than ξ , the interface can be described by a single-valued height function, which in dimensions $1 < d < 3$ is a self-affine fractal with $\alpha = (3-d)/2$ (in pure systems). In this context, the limit $\alpha=0$ corresponds to a smooth interface, since the width remains microscopically small even as $L \rightarrow \infty$ [13]. For $\alpha > 0$, the interface is termed “rough,” since the width diverges as $L \rightarrow \infty$. The upper limit $\alpha=1$ corresponds to an interface so convoluted that it actually “fills out” the entire bulk, d -dimensional volume [11]. Within this context, larger values of α correspond to rougher interfaces.

The paradox is thus resolved by taking note of which limit is envisioned in the case at hand: $L \rightarrow \infty$, or $L \rightarrow 0$. The former viewpoint is more natural to capillary-wave and other physical phenomena associated with liquid-gas interfaces, while the latter viewpoint is more readily associated with local atomic rearrangements which can occur on the surfaces of solid materials.

In conclusion, an increase in the roughness exponent may imply either an increase or decrease in the perceived surface “roughness.” The roughness exponent quantifies how the roughness *changes* with length scale, but is not a measure of the roughness itself. It is perhaps better referred to as a *relative*, or *comparative* roughness exponent.

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