Fractal Dimension of Rough Surfaces in the Solid-on-Solid Model

A recent Letter by Mon[1,2] reported Monte Carlo simulations of rough surfaces in the solid-on-solid (SOS) model[3,4] for spatial dimensions $d=2$ and 3. The aim of the work is to determine the fractal dimension D of these surfaces. His numerical data show that the excess surface area A measured with a length resolution L has a power-law dependence $A(L)\simeq L^{d-1-D}$, where[1] $D=1.58\pm0.06$ for $d=2$ and[2] $D=3.25\pm0.05$ for $d=3$. The purpose of this Comment is to point out that this problem has recently been studied by another method and different results obtained.[5,6]

The SOS model[3,4] is inherently anisotropic because there are only vertical fluctuations above a flat basal plane. In the rough phase, the vertical root-mean-square width of the interface, w, diverges with increasing length L in the basal plane as a power law:

$$w\simeq b(L/b)^{x}. \tag{1}$$

The characteristic length b defines a crossover length, because when $L=b$, then $w=L$.[5] Such surfaces have different rescaling factors along different spatial directions and are called *self-affine* fractals,[7] as opposed to *self-similar* fractals, which are isotropic. The fractal dimension is given by[5,7] $D=d-x$. This is due to the fact that the excess surface area on length scale L can be estimated as

$$A(L)\simeq A_0 w/L\simeq A_0(b/L)^{1-x}, \tag{2}$$

where A_0 is the area of the basal plane above which fluctuations occur. Note that for $L\ll b$, $A(L)\gg A_0$. The identification of the exponent $x-1$ with $d-1-D$ gives $D=d-x$. Note also, from Eq. (2), that for $L\gg b$ the surface becomes effectively smooth, since $A(L)\ll A_0$.

It is well established theoretically that the SOS model has $x=\frac{1}{2}(3-d)$ for $d\leq 3$, with $w\sim(\ln L)^{1/2}$ for $d=3$.[3,4] Hence $x=\frac{1}{2}$ and 0 for $d=2$ and 3, respectively, which implies $D=\frac{3}{2}$ for $d=2$ and $D=3$ for $d=3$. The $d=2$ result is exact and easily derived.[8] A completely general SOS model in $d=2$ has energy E given by $E/k_BT=K\sum_i f(|h_i-h_{i+1}|)$, where the "column heights" $\{h_i\}$ are integers and $f(x)$ is an arbitrary function. For "free" boundary conditions (periodic boundary conditions are only slightly more complicated, and the final result is the same) the model is solved by the introduction of the difference variables $n_i\equiv h_i-h_{i+1}$. Then each n is an independent variable with probability distribution $P(n)=z^{-1}\exp\{-Kf(|n|)\}$, where $z=\sum_{n=-\infty}^{\infty}\times\exp\{-Kf(|n|)\}$ is the one-variable partition function. By the central-limit theorem, the distribution $P(h_L)$ of the variable $h_L\equiv h_i-h_{i+L}=\sum_{j=i}^{i+L-1}n_j$ approaches for large L a Gaussian form with standard deviation $w=\langle h_L^2\rangle^{1/2}=L^{1/2}\langle n^2\rangle^{1/2}$. Thus, $x=\frac{1}{2}$ for $d=2$. For $d=3$, the result $w\sim(\ln L)^{1/2}$, i.e., $x=0$, follows from the properties of the two-dimensional XY model in the low-temperature phase.[3]

Mon's result for $d=2$ is consistent with these analytic predictions, but there is a larger discrepancy for $d=3$. In particular, the latter result violates the inequality $D\leq d$ that follows from Eq. (1): x cannot be less than zero because physical fluctuations increase with increasing distance.

Our analytic considerations differ from Mon's numerical calculation in two technical respects. First, he calculated $\langle|h_L|\rangle$ instead of $\langle h_L^2\rangle^{1/2}$. We believe this has no effect on x or D for the following reason. We have shown that, for $d=2$, $P(h_L)$ has the scaling form $P(h_L)=L^{-x}g(h_L L^{-x})$, with $x=\frac{1}{2}$. This should hold for other dimensions, with different values of x, so that $\langle|h_L|\rangle$ and $\langle h_L^2\rangle^{1/2}$ both scale as L^x. Second, the height difference calculated by Mon is rounded off according to the resolution L. As a result, his measured area is always less than the true area. The difference increases with increasing L, which tends to give a larger value for D.

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[1]K. K. Mon, Phys. Rev. Lett. **57**, 866 (1986).

[2]K. K. Mon, Phys. Rev. Lett. **57**, 1963(E) (1986). This Erratum corrects the value of D for $d=3$ given in Ref. 1.

[3]For a review, see J. D. Weeks, in *Ordering in Strongly Fluctuating Condensed Matter Systems,* edited by T. Riste (Plenum, New York, 1980).

[4]See, e.g., D. J. Wallace, in *Phase Transitions, Cargese 1980,* edited by M. Levy, J. C. Le Guillou, and J. Zinn-Justin, NATO Advanced Studies Institute, Series B, Vol. 72 (Plenum, New York, 1982).

[5]P.-z. Wong, J. Howard, and J.-S. Lin, Phys. Rev. Lett. **57**, 637 (1986).

[6]P.-z. Wong, Phys. Rev. B **32**, 7417 (1985).

[7]See, e.g., R. F. Voss, in *Scaling Phenomena in Disordered Systems,* edited by R. Pynn and A. Skjeltorp (Plenum, New York, 1985).

[8]See, e.g., H. J. Leamy, G. H. Gilmer, and K. A. Jackson, *Surface Physics of Materials,* edited by J. M. Blakely (Academic, New York, 1976), p. 121.