# Self-Similarity and Fractal Dimension of a Roughening Interface by Monte Carlo Simulations

K. K. Mon
*Exxon Production Research Company, Houston, Texas 77001*
(Received 10 February 1986)

It is shown by Monte Carlo simulations that the area of an interface in two and three bulk dimensions as modeled by a discrete solid-on-solid model above the roughening transition is self-similar over a wide range of length scales. The fractal dimensions are estimated for the first time to be $2.8 \pm 0.03$ and $1.58 \pm 0.06$ for three and two dimensions, respectively. Additional Monte Carlo simulations of two-dimensional Ising lattice-gas interfaces have also been performed and are consistent with the solid-on-solid results.

PACS numbers: 68.35.Fx, 64.60.Ak, 68.35.Bs, 73.40.−c

Surface roughness and interfacial disorders are topics of broad fundamental and applied interest, relevant to a wide range of physical phenomena. Some important examples are the electrical transport properties at interfaces between two different media,[1] adsorption and diffusion on surfaces,[2] crystal growth,[3] wetting,[4] and pore surface of rocks.[5] Recent progress has shown that a useful quantitative description of a wide range of surface and interfacial disorders can be obtained in terms of self-similarity over a range of length scales and the related fractal dimension.[6] One important property of surfaces and interfaces[6] is the amount of area $\mathcal{A}(L)$ measured on different length scales $L$. For an interface in $d$ bulk dimensions, we have

$$\mathcal{A}(L) \sim L^{-(D-d_f)} \tag{1}$$

for $l_1 < L < l_2$ and $d_f = d-1$. $l_1$ and $l_2$ are the limits of self-similarity and $D$ is the fractal dimension. $D$ has been measured experimentally[2,5] and exhibits values of $2 \leq D < 3$ for $d=3$ systems. Low values of $D$ are associated with rather smooth, flat surfaces while larger values represent more complicated space-filling surfaces.

A complete detailed understanding of the origin of such wide ranges of interfacial disorders does not yet exist. It is a complex physical problem which depends on both the physics and chemistry of the growth process in the formation of the interfaces. Theoretical and numerical studies of rather simple growth models have contributed toward progress in such understanding.[7] One such model which has been studied extensively in recent years[7-9] has been the discrete solid-on-solid (SOS) model of the crystal-melt interface. It is now widely accepted that the model has a roughening transition temperature, $T_R$, above which the interface changes from smooth to rough.[7] Although there are numerous computer-simulation studies[7] of the SOS model aimed at clarifying the nature of the roughening transition, to our knowledge, evidence for self-similarity and estimates for the fractal dimension have not yet been reported.

In this paper, a Monte Carlo study of the nature of the roughness of the interface above the roughening temperature is presented for $d=3$ and 2. It is shown that the roughening surface is self-similar over a wide range of length scales and the area density has a well-defined fractal dimension of $2.8 \pm 0.03$ and $1.58 \pm 0.06$ for $d=3$ and 2, respectively. The amplitude of the roughness scales linearly with the temperature. Additional Monte Carlo simulations of two-dimensional Ising lattice-gas interfaces have also been performed and are consistent with the SOS results

A standard discrete solid-on-solid model of two coexisting phases in three dimensions[7,8] is a two-dimensional lattice of columns with integer heights $h_i$ ($-\infty < h_i < \infty$). (For $d=2$, it is a chain.) The SOS model ignores overhangs and bubbles and is used extensively in various modifications of studied interfaces.[7] In my Monte Carlo simulations, a square lattice of $N \times N$ columns (with lattice constant $w=1$) is considered (extension to $d=2$ is straightforward). The energy $E$ of a given configuration of $h_i$ at temperature $T$ is taken as

$$E/k_B T = K \sum_{\langle i,j \rangle} |h_i - h_j| \tag{2}$$

with Boltzman constant $k_B$ and reduced coupling $K$ ($=J/k_B T$). The sum is over nearest neighbors and $J$ plays the role of an effective interfacial tension. The roughening transition occurs for $K^{-1} \sim 1$ and 0 for $d=3$ and 2, respectively. The energy $E$ is also related to the excess area $\mathcal{A}_{ex}$, which is defined to be the increase in surface area due to excitations and can be considered to be a measure of the roughness. The ground state is flat and has zero energy and excess area. The total area of the flat ground state (in units of the lattice constant, $w=1$) is $N^2$. We define the ensemble-averaged excess area density as

$$A(L) = \langle \mathcal{A}_{ex}(L) \rangle / N^2 = \langle \mathcal{A}_{total}(L) \rangle / N^2 - 1. \tag{3}$$

The area density $A(L)$ is measured on a different length scale ($L$) and averaged over equilibrium config-

urations generated by standard Monte Carlo techniques.[7] To obtain $A(L)$, we average out the details of the configurations with a length scale less than $L$. [The lattice is divided into cells of size $L \times L$. An average column height in units of $L$ is obtained for each cell and used to calculate the excess area density $A(L)$. This definition is computationally efficient and suffices for this first calculation. An alternative definition will be considered elsewhere.] $A(L)$ is thus a measure of excitations with length scale larger than or equal to $L$. The configurations of column heights are generated by a standard biased random walk in phase space with a probability governed by the Boltzmann distribution.[7] (About 40000 Monte Carlo steps per site with periodic boundary conditions are used.) A range of couplings ($K$) and system sizes ($N$) have been considered for both $d=3$ and 2. The excess area density $A(L)$ is self-similar over a wide range of length scales (see Figs. 1 and 2). The amplitude of roughness scales with the temperature $T$ or $K^{-1}$. The slope of the log-log plot in Fig. 1 is $0.8 \pm 0.03$ for $d=3$ and provides an estimate of the fractal dimension $D=2.8 \pm 0.03$. [See Eq. (1).] For $d=2$, the slope is $0.58 \pm 0.06$ and $D=1.58 \pm 0.06$. The error is estimated from the scatter of the data points. An approximate description of our results is

$$A(L) \sim K^{-1} L^{-0.8} \quad \text{for } d=3,$$
$$A(L) \sim K^{-1} L^{-0.58} \quad \text{for } d=2. \tag{4}$$

For lower temperatures (larger $K$), both the amplitude and regime of self-similarity are reduced. Because a lattice is used in the model, the lower limit ($l_1$) is bounded by the lattice spacing. The upper limit [$l_2(N)$] for large systems near the thermodynamic limit ($N=\infty$) should depend only on the temperature. For small system sizes [$N < l_2(N=\infty)$], long-wavelength excitations are prohibited. The upper limit $l_2(N)$ to scaling decreases as the size $N$ decreases. See Figs. 1 and 2 (for $K=0.002$ and $K=0.02$, respectively). The fractal dimension $D$ is the same within the accuracy of the simulations for a given bulk dimension and raises the possibility of universality for $D$. A standard test for universality would be to consider different lattices, such as the triangular lattice for $d=3$. I have considered perhaps a stronger test for universality by considering a Monte Carlo simulation of the full Ising lattice-gas model with an interface.

Monte Carlo simulations of a two-dimensional Ising lattice gas with an interface have been performed to probe the universality of the SOS model results. A square lattice with $M$ columns and $N$ rows ($240 \times 80$ and $240 \times 40$) has been considered for temperature $T=0.5$ and 0.7, in units of $T_c$.[10] Top- and bottom-row spins are coupled to pinned spins to impose an interface for $T < T_c$. Periodic boundary conditions are used for the other two sides. At these temperatures,

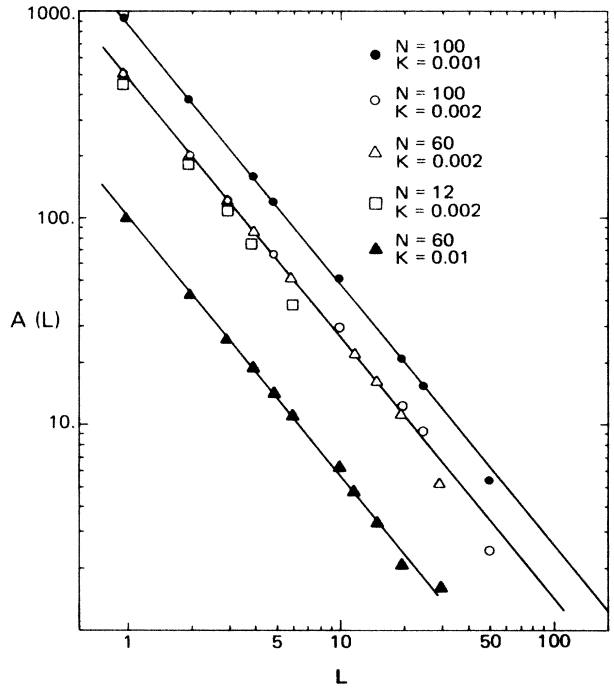


FIG. 1. Log-log plots of Monte Carlo results for the excess area density $A(L)$ for different system sizes ($N \times N$) and couplings ($K$), measured on length scale $L$ for the two-dimensional SOS model. The solid line is a fit with slope of 0.8 indicating a fractal dimension of 2.8. Bulk dimension ($d$) is 3.

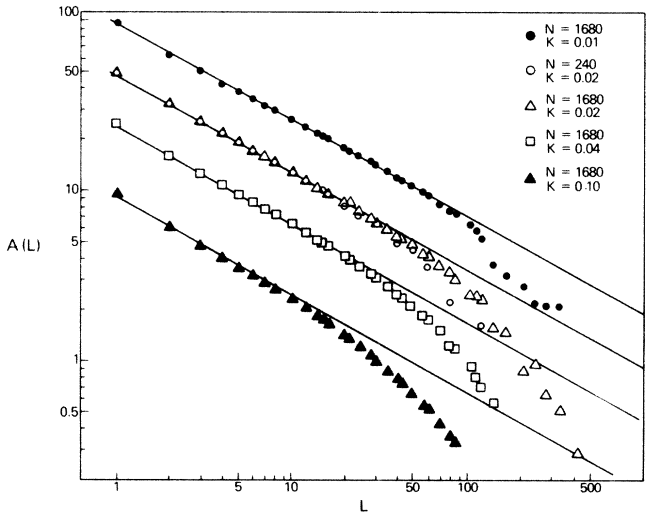


FIG. 2. Log-log plots of Monte Carlo results for the excess area density $A(L)$ for different system sizes ($N$) and couplings ($K$), measured on length scales $L$ for one-dimensional SOS model. The solid line is a fit with slope of 0.58 indicating a fractal dimension of 1.58. Bulk dimension ($d$) is 2.

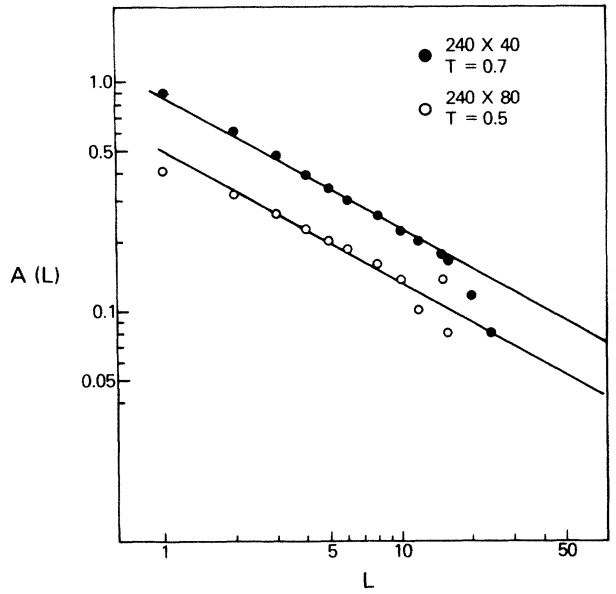


FIG. 3. Log-log plots of Monte Carlo results for the excess area density $A(L)$ for two-dimensional Ising square lattice with an interface (see text). Temperature $T$ is in units of $T_c$. The solid line is a fit with slope of 0.58, consistent with the SOS results.

well-defined interfaces are observed. The excess area density is shown in Fig. 3. Self-similarity and fractal dimension is consistent with the SOS results. This provides support for the possibility of universality for the fractal dimension. Similar simulations for $d=3$ are under considerations.

The observation of self-similarity for the roughening interface is possible because the SOS models are in the critical phase at and above the roughening transition. Critical systems exhibit fluctuations on all length scales and can be self-similar. The demonstrations of self-similarity by computer simulation and the measurements of the fractal dimension, to my knowledge, are new and have a number of important implications. First, these results raise the possibility that surface self-similarity in some physical systems may be related to dynamical formation conditions favorable to the freezing in of an equilibrium configuration of systems above the roughening transition. Further theoretical and experimental investigations to probe this possibility may lead to new insights and understanding. Second, since the SOS model has been shown to be a successful approximation in modeling wetting films,[11] two observations follow: The surface of the wetting films above roughening is self-similar, and interfacial adsorption[12] is in fact adsorption onto a surface fractal. Third, my simulation indicates that the SOS model provides a convenient and well-controlled technique for generating surface fractal with known roughness amplitude and fractal dimension. This should be useful for other simulations, investigating various static and dynamic physical phenomena associated with self-similar surfaces.

The author has benefitted from Dr. A. H. Thompson and the Exxon Production Research Rock Physics Group. He thanks them.

[1]For a recent example, see S. H. Liu, Phys. Rev. Lett. **55**, 529 (1985), and references therein.

[2]D. Avnir, D. Farin, and P. Pfeifer, Nature (London) **308**, 261 (1984); P. Pfeifer, D. Avnir, and D. Farin, J. Stat. Phys. **36**, 699 (1984), and references therein. See also *Wetting, Spreading, and Adhesion,* edited by J. F. Padday (Academic, New York, 1978).

[3]For introduction and references, see D. Elwell and H. J. Schell, *Crystal Growth From High Temperature Solution* (Academic, New York, 1975).

[4]P. G. de Gennes, Rev. Mod. Phys. **57**, 877 (1985), and references therein.

[5]A. J. Katz and A. H. Thomspon, Phys. Rev. Lett. **54**, 1325 (1985).

[6]B. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, San Francisco, 1982).

[7]See for recent reviews *Monte Carlo Methods in Statistical Physics,* edited by K. Binder (Springer, Berlin, 1979); *Applications of Monte Carlo Methods,* edited by K. Binder (Springer, Berlin, 1984). For reviews on critical properties of surfaces and interfaces, see David Jasnow, Rep. Prog. Phys. **47**, 1059 (1984); K. Binder, *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983).

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

[9]For example, see R. H. Swendsen, Phys. Rev. B **15**, 5421 (1977); H. J. Leamy, G. H. Gilmer, and K. A. Jackson, in *Surface Physics,* edited by J. H. Blakeley (Academic, New York, 1976). For experimental observation of roughening, see K. A. Jackson and C. E. Miller, J. Cryst. Growth **40**, 169 (1977). For recent papers on the effect of randomness, see D. A. Huse and C. L. Henley, Phys. Rev. Lett. **54**, 2708 (1985); M. Kardar and D. R. Nelson, Phys. Rev. Lett. **55**, 1157 (1985); D. A. Huse, C. L. Henley, and D. S. Fisher, Phys. Rev. Lett. **55**, 2924 (1985); M. Kardar, Phys. Rev. Lett. **55**, 2923 (1985).

[10]L. Onsager, Phys. Rev. **65**, 117 (1944).

[11]For example, see M. P. Nightingale, W. F. Saam, and M. Schick, Phys. Rev. Lett. **51**, 1275 (1983); E. Brezin, B. I. Halperin, and S. Leibler, Phys. Rev. Lett. **50**, 1387 (1983); and Ref. 4.

[12]For example, see the review by W. Selke, in *Static Critical Phenomena in Inhomogeneous Systems,* edited by A. Pekalski and J. Sznajd, Lecture Notes in Physics Vol. 206 (Springer, New York, 1984).