Computer simulation for the roughness and fractal properties of film surfaces

Mitsunobu Nakamura
Department of Electronic Engineering, Tamagawa University, Machida, Tokyo 194, Japan
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Physical properties of films deposited on substrates and the fractal nature of film shapes have been topics of widespread interest. However, the fractal property of the roughness of film surfaces is little studied. In this paper we investigate, by computer simulation, the fractal behavior of one-dimensional random surfaces, as a first approach to this topic. Here, random surfaces are shaped by depositing unit-square particles one by one at random on segments divided into unit cells, and we plot the surface lengths of clusters formed on the segments against the areas. As a result, we have obtained evidence that the clusters exhibit two typical fractal dimensions (1.46 and 1.86).

Many physical properties of films are directly addressed by the two-dimensional continuum percolation problem. We studied, by computer simulation, the two-dimensional continuum percolation problem,[1,2] and found that the critical metallic area fractions for the metal-insulator transition agreed well with those of actual measurements.[3,4] Following this earlier work, we have studied the fractal nature[5–7] of two-dimensional continuum percolation clusters, and these results also agreed well with actually observed fractal properties of metal films deposited on substrates, using transmission micrograph and image processing by computer.[4,8,9] However, the fractal property of the roughness of film surfaces has to date received little attention. Here as a first approach to the problem, we apply a computer simulation, and treat the problem in one dimension, i.e., we study the roughness and fractal of the section normal to the film surface.

First we present a basic model of random surfaces for computer simulation. We fill unit-square particles on a segment with length N divided into unit cells, at random, one by one. We present in Fig. 1 an example of a pattern for $N=100$ formed in the course of the deposition. This model is a normal section of random deposition of unit-cubic particles on a square mesh.

The fractal dimension D_f may be defined in various ways.[10] In our previous papers[5–7] we used (1) for the two-dimensional continuum percolation problem

$$P=cA^{D_f/2}, \tag{1}$$

where P is the perimeter of fractal objects, c is a proportional constant, and A is the area. Lovejoy[11] also used (1) to estimate the fractal dimension of cloud and rain area boundaries. Here we apply (2), which modifies (1) by replacing P with L,

$$L=cA^{D_f/2}, \tag{2}$$

where L is the surface length of clusters.

In Fig. 2, we plot L against A for the length $N=100\,000$. Figure 2 obviously shows that the fractal property exists and that the fractal dimensions are different according to the two sizes of clusters (small and large). Applying the least-squares method, we fit the two straight lines in Fig. 2, and present c, D_f, and the correlation coefficient γ:

$$c=2.68, \tag{3}$$

$$D_f=1.46, \tag{4}$$

$$\gamma=0.980 \tag{5}$$

FIG. 1. An example of patterns formed on a segment divided into 100 unit cells ($N=100$).

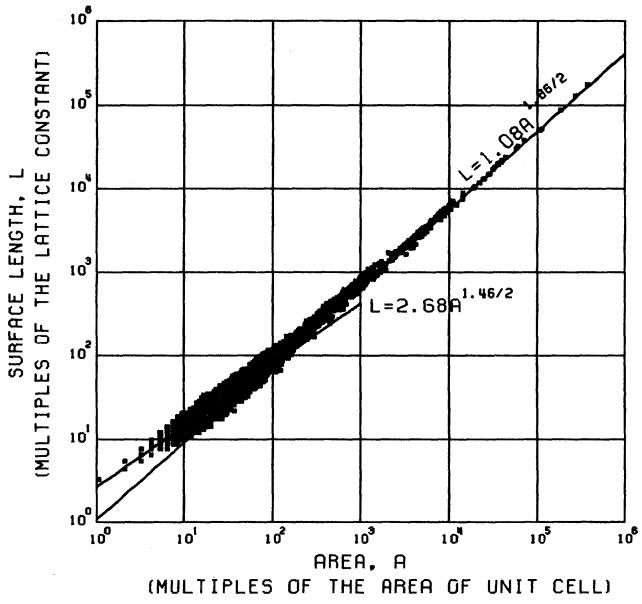

FIG. 2. Scatter plot of the surface length L vs area A for the base length $N=100\,000$.

for small clusters, and

$$c = 1.08 , \tag{6}$$

$$D_f = 1.86 , \tag{7}$$

$$\gamma = 0.998 \tag{8}$$

for large clusters.

The clusters with $D_f = 1.46$ are small clusters, and the data points fluctuate, but the correlation coefficient γ (equal to 0.980) is very close to unity, therefore, the fitting of the straight line is proper, and the value of the fractal dimension is significant.

The clusters with $D_f = 1.86$ are large and rapidly growing clusters which absorb or unite other clusters. Although the clusters are formed on a one-dimensional segment, it is natural that the rapid growth takes place when we consider that their forms are two dimensional and are normal sectional shapes of rapidly growing three-dimensional percolation clusters deposited on planes. In fact the value (1.86) of the fractal dimension is very close to that (1.9) for the two-dimensional continuum percolation clusters.[4–9]

However, the value (1.86) is far greater than the fractal dimensions of other boundary shapes such as clouds (1.35, Ref. 11) and coast lines (1.25).[10] It means that the surface of the model in this paper is much rougher than other boundary surfaces. The reason is that in this model rigid particles are deposited and no particles deform and move after the depositions for the surface to become smooth.

Although here we have carried out a simple computer simulation for formation of film surface, we can predict that when we observe the normal section of actual metal films two typical irregular surfaces appear. One of the types is a group of small clusters, and the fractal dimension is smaller. Another type is a group of large clusters, and the fractal dimension is larger. However, in actual surfaces, deposited bodies are soft, and they deform and move after the depositions for the film surface to become smooth. Hence their fractal dimensions are much smaller than the model in this paper. In view of this, further computer simulations for the formation of film surfaces will be necessary. With the aid of computer simulations, one might one day be able to predict what operations are required to obtain smooth surfaces.

In summary, we have studied the fractal property of a random surface model with use of computer simulation. The random surface was formed by putting unit-square particles one by one at random on a segment divided into unit cells. The fractal dimensions of clusters formed are 1.46 and 1.86, respectively, for small clusters and for the growing, larger clusters. These fractal dimensions indicate well the classification of the shapes of clusters generated in the process of a deposition. The fractal dimension 1.86 agrees well with that (1.9) of the two-dimensional percolation clusters.

In the present work, we carried out by computer simulation a study of only the simplest one-dimensional surface formation. Further work on two-dimensional and more complicated problems is now in progress.

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