Quasi-two-dimensional diffusion-limited aggregation

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We have carried out Monte Carlo simulations to investigate the effects of quasi-twodimensional systems on the aggregate. We find that the ratio of height to width is responsible for the morphology of the generated cluster, and, when the ratio exceeds 0.12, the ramified structure disappears and the aggregate becomes compact.

Diffusion-limited aggregation (DLA) proposed by Witten and Sander¹ is a two-dimensional model. However, in many actual cases the aggregation occurs in quasi-twodimensional space; i.e., there is a small height along the third dimension. The fact that a small height exists will greatly affect the morphology in the aggregation processes and, therefore, should be taken into account.

We have carried out Monte Carlo simulations to investigate the effect of quasi-two-dimensional aggregation on a $200 \times 200 \times H$ cubic lattice, where H is the height along the third dimension and is tunable. The diffusive particles are allowed to move in the quasi-two-dimensional volume, while the aggregated cluster is strictly restricted to a twodimensional space (surface cluster). In this work H=1 (exactly as in DLA), 3, 8, and 16. The ratios of height to width for H=1, 3, 8, and 16 are 0.005, 0.015, 0.04, and 0.08, respectively. At the beginning a seed is placed at the center of the bottom layer of lattices and the aggregate will develop on this plane. Our model is identical to DLA except in the following cases: (i) When the random walker is on the upper or lower surface, the moving which makes the walker leave the lattices will be disallowed; (ii) the moving of the random walker from the next-to-the-bottom layer to the bottom layer is permitted if and only if the site on the bottom layer has not been occupied by the aggregate; (iii) when the walker goes to one of the nearest

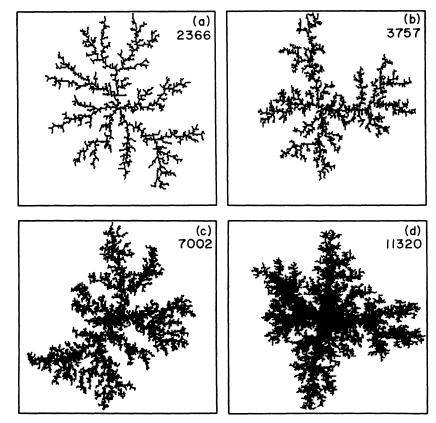


FIG. 1. Aggregated clusters in quasi-two-dimensional diffusion-limited aggregation with different heights. (a) H=1 (DLA), (b) H=3, (c) H=8, (d) H=16.

sites of the aggregate and is on the bottom layer, it becomes part of the cluster.

Applying this model we obtained the results shown in Fig. 1. Using the sandbox method,² the fractal dimension D was measured and we have $D=1.65\pm0.03$, 1.72 ± 0.02 , 1.76 ± 0.02 , and 1.90 ± 0.01 for H=1, 3, 8, and 16 or a height-width ratio equal to 0.005, 0.015, 0.04, and 0.08, respectively. From the figure, we learn that when the ratio increases, the cluster becomes more compact. When H=24, the formed pattern shows no ramified structure and the fractal dimension is two. This reflects a height-to-width ratio of 0.12. If a ratio exceeds this value, quasi-two-dimensional diffusion will produce a compact aggregate.

One thing should be mentioned in the case of quasitwo-dimensional diffusion aggregation. In the twodimensional DLA model, the existing cluster prevents the newly arriving particles from penetrating the cluster; i.e., the entering particles are strongly screened by the cluster.¹ Therefore, the generated cluster has an open structure and is highly ramified. In our case, when one observes that along the projective direction the particle "contacts" the cluster, it does not mean that there is a real contact, unless the particle is on that plane. Thus, because of the small height along the third dimension, the screening effect by the existing cluster is relatively small and the cluster can be more compact.

In the experiment performed by Hou and Wu on a-Ge/Au bilayer thin-film aggregation,³ it was found that the Ge atoms aggregate to form a cluster, and the fractal dimension increases with the rising in annealing temperature. In their case, Ge atoms diffuse much faster in polycrystalline Au than in themselves, and we can find out the similarities between the experiment and this quasi-twodimensional model. The annealing temperature (T_a) in their experiment plays the same role as H. When T_a rises Ge atoms stay on the sites where they first contact the cluster and continue to diffuse in quasi-two-dimensional space. We have learned from the above discussion that the existing two-dimensional cluster will screen the particles diffusing in quasi-two-dimensional volume less, and it is certain that the cluster will be more compact when the temperature rises. Moreover, we noticed that a critical temperature exists in their experiment and if the temperature exceeds that point, the clusters are compact. Another reason for this is that when T_a rises, the nucleation probability amplifies. As a result, each nucleus attracts fewer particles, and the size of the formed cluster decreases. This indicates an increment in the height-to-width ratio. Therefore, the aggregated cluster becomes more compact and has a higher fractal dimension.

¹T. A. Witten and L. M. Sander, Phys. Rev. B 27, 5686 (1983). ²S. R. Forrest and T. A. Witten, J. Phys. A 12, L109 (1979). ³J. G. Hou and Z. Q. Wu, Phys. Rev. B 40, 1008 (1989).