Aggregate models of pattern formation

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(Received 5 September 1985)

A one-parameter generalization of the diffusion-limited-aggregation (DLA) model, originally suggested by Witten and Sander, is studied. On changing the parameter, the resulting aggregate geometry changes from a fractal DLA-like structure to a compact one. Along the way, geometrical structures bearing a striking resemblance to viscous fingers and a variety of aggregates found in nature are obtained.

There has been a great deal of recent theoretical and experimental interest in the study of shapes of patterns formed in diverse systems such as the growth of viscous fingers in a Hele-Shaw cell,[1,2] two-phase fluid flow in porous media,[3] electric breakdown,[4] irreversible kinetic aggregation of gold colloids,[5] and the sputter deposition of thin films of $NbGe_2$.[6] It has been argued that diffusion-limited aggregation[7] (DLA) is the underlying physical mechanism responsible for fractal geometries[8] in many of these systems. In the standard DLA simulation, a seed particle is placed at one point on a lattice. Then a random walker is introduced into the system. When it comes to a nearest-neighbor site it becomes part of the cluster and a new random walker is introduced. By repeating this procedure, a very ramified structure is obtained.

In this paper we present a detailed study of a simple one-parameter generalization of the Witten-Sander DLA model.[7] The generalized model contains a parameter $0<\alpha\leq 1$, which controls the surface structure. On changing the parameter α from 1 to 0, the resulting geometry changes from a fractal DLA-like structure to a compact one. Along the way, geometrical structures bearing a striking resemblance to many observed in nature are found.

In a recent paper Vicsek[9] considered the effects of surface tension on the DLA-like simulation. He assumed that the sticking probability of the random walker to the growing aggregate depended on the local curvature. Since the local curvature is a macroscopic quantity, his work is in the spirit of simulating continuum equations using the Monte Carlo method on the lattice.[10] However, in order to avoid obtaining a ramified cluster, a microscopic rule is added: After sticking to the cluster the particle relaxes to the neighboring site which has the largest number of bonds connected to the cluster.

We reconsider an earlier model due to Witten and Sander[11] involving only microscopic interactions on the surface. The focus of our analysis and our results are, however, different from theirs. Briefly, their model starts with the DLA model and adds the following important modification: When a new particle makes contact with the growing cluster it does not necessarily "stick." Instead, the sticking probability p depends on B, the number of nearest-neighbor occupied sites in the cluster. For a square lattice (on which we have carried out all of our simulations), the sticking probability is

$$p=\begin{cases}1 & \text{if } B=3,\\ \alpha & \text{if } B=2,\\ \alpha^2 & \text{if } B=1\ .\end{cases} \tag{1}$$

The standard DLA case corresponds to $\alpha=1$, whereas the limit $\alpha\to 0$ leads to compact structures because holes with $B=3$ will have a much higher tendency to fill than points with $B=1$. Even though Eq. (1) is a microscopic rule, we expect that it generates surface tension at a macroscopic length which may, for example, be represented by the Gibbs-Thomson relation. Therefore the parameter α can be regarded as a measure of the surface tension.

How do the patterns of the clusters evolve as α changes from 1 to 0? To answer this question and to make qualitative contact with experimental results, we have carried out extensive computer simulations in two distinct geometries. The first of these is the rectangular geometry shown in Fig. 1 with seed particles present all along the width of the cell. We assume periodic boundary conditions in the transverse direction. The second geometry corresponds to the conventional radial geometry with one seed particle at the origin. In the event that an incoming particle does not stick to the growing cluster, we let it continue walking in the region external to the cluster, i.e., we do not let the incoming particle penetrate the cluster.

To characterize the resulting patterns quantitatively, we have studied two different fractal dimensions. The first of these is the conventional bulk fractal dimension D_b defined by the relationship between the mass M (number of particles) and the radius of gyration R:

$$M\approx R^{D_b} \tag{2}$$

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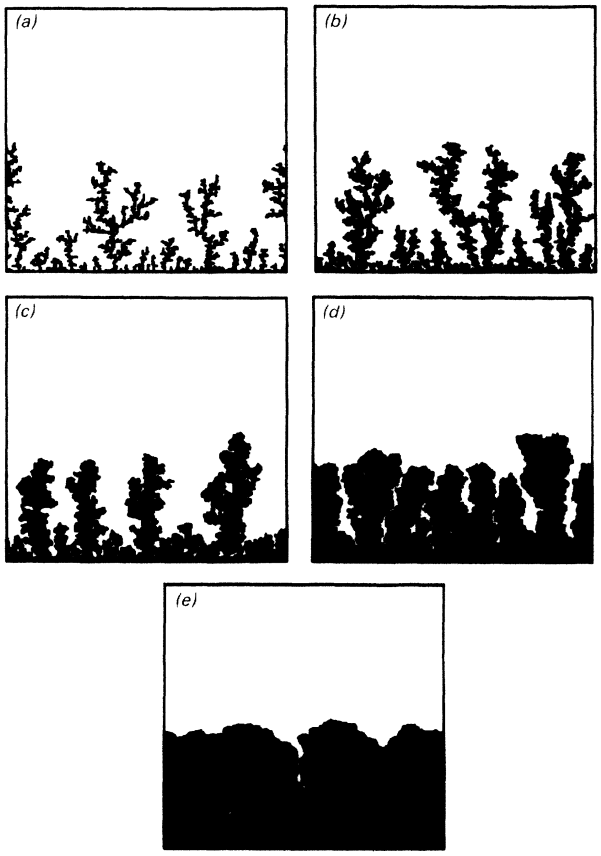

FIG. 1. Clusters grown on a 256×256 lattice in the rectangular geometry. The diffusing particles come in from the top with the seed particles initially located all along the bottom edge. Periodic boundary conditions are assumed along the side walls. The values of α are (a) 1.0, (b) 0.4, (c) 0.2, (d) 0.1, and (e) 0.05.

We have also calculated the fractal dimension of the exterior perimeter length D_p. The total exterior perimeter is measured using rulers with lengths ranging between $L=3.0$ and $L=11.3$ measured in units of the lattice spacing. The apparent length of the fractal curve in units of L decreases as L^{-D_p}. Nittmann *et al.*,[2] in their analysis of the fractal growth of viscous fingers, have argued that D_b and D_p ought to be equal for the DLA cluster ($\alpha=1$). This appears to be in contradiction with their Fig. 6 in which the fractal dimension does not seem to asymptote to the Witten-Sander value as the Hele-Shaw width tends to infinity. Our analysis suggests that even for the DLA cluster $D_b > D_p$ (see Fig. 3).

Figure 1 shows some sample clusters which were grown using the rectangular geometry with dimensions 128×256. Different values of α were used in the different pictures. As α drops from 1, the highly ramified fractal DLA cluster thickens at first. Then fingerlike structures emerge due to the competition between the attractive effects of the surface tension and the screening effects. Eventually, for sufficiently small values of α (≤ 0.05) a flat interface is obtained. A plot of D_p versus α is qualitatively and even quantitatively very similar to that exhibited in Fig. 3 for the radial geometry case. On narrowing the width of the rectangle, D_p is found to decrease in accordance with the finding of Nittmann *et al.*[2]

Figure 2 shows a similar set of clusters which were grown using the radial geometry on a 256×256 lattice. Again, as α drops from 1 the DLA cluster thickens. For intermediate values of α the patterns are not unlike those found in snowflake simulations[12] in the absence of anisotropy. At low values of α the pattern again becomes compact ($\alpha \leq 0.05$). Note that for the $\alpha=0.05$ cluster, the underlying lattice structure plays an important role. In particular, the aggregate interface is substantially flat with small-scale fluctuations. This is not the case for the clusters with $\alpha \geq 0.1$. Between $\alpha=0.05$ and $\alpha=0.1$, there is a definite change of the surface structure in the nonequilibrium kinetic process. It is an important question to ask whether this change occurs as a smooth crossover or abruptly as in a phase transition. In an analogous equilibrium-crystal-shape problem, an abrupt change does take place and is known as the roughening transition.

A plot of D_b and D_p versus α is shown in Fig. 3. It is interesting to note that the dimensionalities seem to be substantially independent of α for values of α greater than

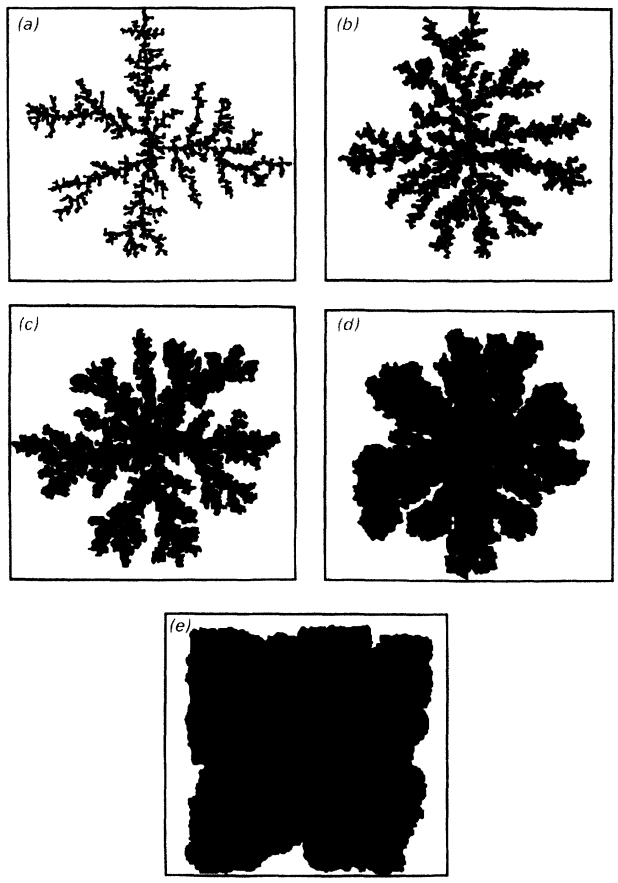

FIG. 2. Clusters grown on a 256×256 lattice in the radial geometry. The diffusion particles come in radially and there is one seed particle initially at the center of the square. The values of α are (a) 1.0, (b) 0.4, (c) 0.2, (d) 0.1, and (e) 0.05.

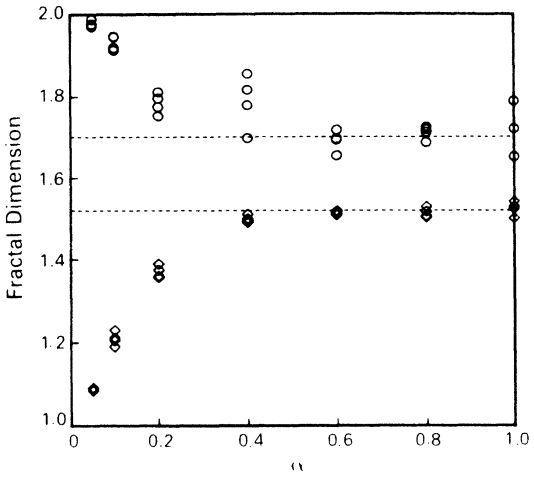

FIG. 3. Fractal dimension versus α in the radial geometry—○ represents D_b and ◇ represents D_p.

approximately 0.4. The crucial point is that the maximum value of D_p is about 1.52 and does not seem to tend asymptotically to the usual DLA-like value around 1.70. As α becomes small, D_b and D_p approach the limiting values 2 and 1, respectively. These are obviously the bulk and perimeter dimensions for a normal compact object in two dimensions.

In conclusion, we have studied a generalized DLA model which extrapolates from a fractal geometry to a compact geometry on changing the value of a surface-tension parameter. As the parameter is varied, clusters are formed with striking resemblances to viscous fingers, tip splitting snowflakes, and a variety of aggregates in nature. It remains an intriguing question whether there are phase transitions for well-defined values of the parameter or whether the geometry evolves continuously. Similar ideas may be useful in understanding facet formation and in studying the kinetic analog of the roughening transition.

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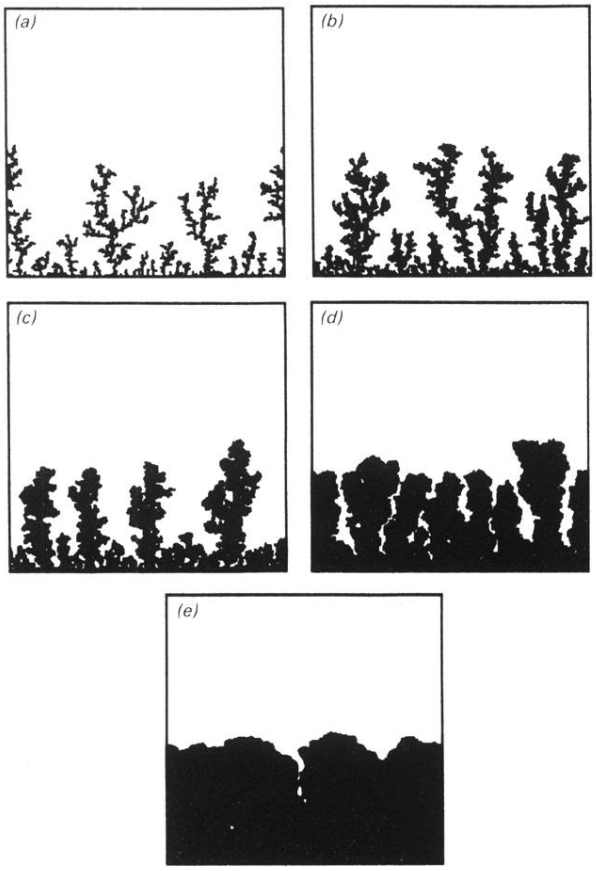

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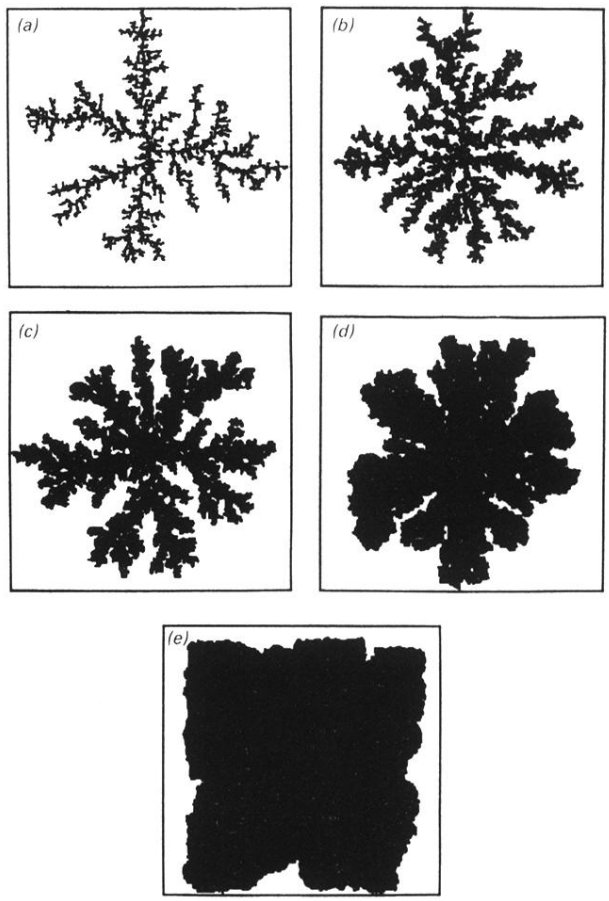

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