

LETTER TO THE EDITOR

Elastic properties of diffusion-limited aggregates

Yacov Kantor and David J Bergman†

Corporate Research Science Laboratories, Exxon Research and Engineering Co, Route 22 East, Annandale, New Jersey 08801, USA

Received 16 July 1985

Abstract. A transfer matrix method has been used to investigate the power law dependence of the effective elastic moduli of a two-dimensional diffusion-limited aggregate on the size l of the aggregate. Scaling exponents have been found to depend on the type of applied deformation. For stretching along the direction of growth the elastic modulus scales as $l^{-2.2 \pm 0.2}$, while for deformations in the direction perpendicular to the direction of growth it is proportional to $l^{-2.8 \pm 0.2}$.

Considerable recent attention has been focused on various properties of diffusion-limited aggregates (DLA) (Witten and Sander 1981, 1983), which provide an adequate description of several physical systems (Brady and Ball 1984, Matsushita *et al* 1984, Nittman *et al* 1985, Elam *et al* 1985). In a standard DLA model a seed aggregate is placed at a lattice site and diffusing particles stick to it and join the aggregate if they visit a neighbouring site to the aggregate. The simplicity and convenience of the model lead to numerous investigations of its physical properties, such as conductivity (Family and Coniglio 1984), mechanical stability (Kantor and Witten 1984), spectral properties (Webman and Grest 1985) and some topological properties (Witten and Kantor 1984, Meakin *et al* 1984). In this letter we report the results of a numerical investigation of the elastic properties of a two-dimensional DLA. Since DLA is a fractal (Mandelbrot 1982) or scale invariant object, its elastic properties have a power law dependence on the linear size l , namely each elastic modulus is proportional to $l^{-\tilde{\tau}}$. We find that the numerical value of the critical exponent $\tilde{\tau}$ depends on the direction of the applied external deformation. For forces which stretch the object along its growth direction $\tilde{\tau} = 2.2 \pm 0.2$, while for forces perpendicular to that direction $\tilde{\tau} = 2.8 \pm 0.2$. This difference in the numerical values of $\tilde{\tau}$ reflects the strong anisotropy in the geometry of DLA.

We use a transfer matrix method (Derrida and Vannimenus 1982) which has been modified by Bergman (1985) to permit the calculation of the effective elastic constants in disordered systems. This method uses an iterative procedure to calculate exactly the elastic response of a system which is defined on a strip of a very large length L and finite width l . The choice of $L \gg l$ produces an effective averaging of the large fluctuations, which are usually present in small $l \times l$ systems, and therefore leads to a highly accurate estimate of the effective elastic constants for each value of l . By shifting one of the long edges of the strip either parallel or perpendicular to the long dimension

† Permanent address: School of Physics and Astronomy‡, Tel Aviv University, 69978 Tel Aviv, Israel.

‡ Supported in part by the Israel Academy of Sciences and Humanities.

of the strip, and by measuring the elastic response (force) we determine the effective values of either the shear modulus $\mu \equiv C_{1212}$ or the 'stretching modulus' $c \equiv C_{2222}$ (the strip is assumed to be parallel to the x axis of the reference frame). The efficiency and accuracy of this method has been demonstrated (Bergman 1985) in the measurement of the critical behaviour of μ and c of a percolating network.

Transfer matrix methods can be applied only to systems whose characteristics do not depend (on the average) on the x coordinate. This, however, is not the case for a regular DLA which is grown from a point seed, since its density decreases with increasing distance from the seed. (From this point of view DLA is more analogous to the infinite cluster of a percolating network at the percolation threshold, viewed from a point which lies on it, than to the entire percolating network, viewed from an arbitrary point.) Therefore, we use a different model, in which a point seed is replaced by a straight line of such seeds. This model has been proposed and investigated by Meakin (1983b) and Rácz and Vicsek (1983). The mass M of such an aggregate scales with the distance h from the surface according to the power law $M \sim h^{D_1}$. This model can be related to the usual DLA. If we assume that the two-point correlation function of a regular DLA (in d dimensions) and the two-point correlation function of a DLA grown from a $(d-1)$ -dimensional surface have the same power-law behaviour then the fractal dimension (Mandelbrot 1982) D_0 of the former is related to the scaling power D_1 of the latter by $D_1 = D_0 - 1$. Thus using the known values of D_0 (Meakin 1983a) we expect a value $D_1 \approx 0.7$.

In our simulation we grew DLA from a line on a two-dimensional triangular lattice (TL). The length L of the starting line (x axis of the coordinate frame) was 10 000. The aggregate was grown in the y direction, and periodic boundary conditions were assumed in the x direction. We used the following Monte Carlo procedure. A particle was released at a random x , at a height y greater than the maximal extent of the aggregate in the y direction. The particle then performed a random walk until it either arrived at a point adjacent to the aggregate and stuck there, becoming a part of the aggregate, or escaped to infinity in the y direction and was eliminated (in the simulation this occurred if $y > L$). This process was repeated until the mass of the aggregate became 150 000, i.e. 15 particles per point of the starting line. The maximal extent of the aggregate in the y direction was 244, its RMS height was 84, and the average height of a particle in the aggregate was 67. (Distances in the y direction are always given in numbers of layers of the TL, i.e. the unit is $\sqrt{2}$ times smaller than the lattice constant which is used to measure distances in the x direction.) Figure 1 depicts part of the aggregate grown from a line in this way. The scaling power measured from the density profile of the aggregate is $D_1 \approx 0.75$. This result is consistent with a previously measured value (Meakin 1983b) and is close to the expected value of D_1 . Usually we can expect a crossover to one-dimensional behaviour when the size of the aggregate becomes comparable with L . However in our simulation we are two orders of magnitude away from that crossover. Although in our calculations we use only the part of the aggregate



Figure 1. A portion of the aggregate grown on a triangular lattice starting from the bottom line. Only the first 80 layers are shown. The tick marks are separated by 50 lattice constants.

where $y \leq 80$, we in fact grew it to a considerably greater height, because the diffusing particles penetrate quite deeply into the aggregate and we wanted to ensure that the entire region $y \leq 80$ had already completed its growth. Even so, 5% of the last 30 000 particles that were released managed to penetrate into that region and increased its total mass by about 1%.

We assume that each occupied site of the TL has three bonds attached to it symmetrically (\blacktriangle), where the length of each bond is $1/\sqrt{3}$ lattice constants of the TL. Thus two neighbouring sites are connected not by a straight line but by two bonds which meet at a 120° angle. If such bonds had been drawn from all the sites of the TL they would form a honeycomb lattice, and the sites of the original TL would occupy alternating sites of the honeycomb lattice. In order to calculate the elastic properties of the aggregate we apply the same Hamiltonian which was used to represent the elastic behaviour of a percolating network (Kantor and Webman 1984). Each bond accounts for an elastic energy $\frac{1}{2}k(\delta b)^2$, where δb is the elongation of the bond, while a pair of adjacent bonds accounts for an elastic energy $\frac{1}{2}m(\delta\phi)^2$, where $\delta\phi$ is the change in the angle between the bonds. These microscopic elastic constants, k and m , are related to the bulk and shear moduli of a full lattice, $\kappa_1 = k/2\sqrt{3}$ and $\mu_1 = 2\sqrt{3}/(k+6m)$, respectively.

In the fractal regime, the effective elastic moduli have a power law dependence on the size of the system, i.e. we expect $c \sim l^{-\tilde{\tau}_c}$ and $\mu \sim l^{-\tilde{\tau}_\mu}$. The exponents $\tilde{\tau}_c$ and $\tilde{\tau}_\mu$ were found to coincide in the percolation problem (Bergman 1985), but this need not be the case here. An estimate of these exponents can be obtained from the following considerations (Kantor and Witten 1984). It can be shown (Kantor and Webman 1984) that the force constant of a single very long chain $\sim m/(\mathcal{R}^2 N)$, where N is the number of bonds in the chain ('chemical' length) and \mathcal{R} is the radius of gyration of the chain in the direction perpendicular to the applied force. (Note that the microscopic constant k does not appear.) If the characteristics of the chain have a power law dependence on its linear size l , namely $\mathcal{R} \sim l^\alpha$ and $N \sim l^\delta$, then the force constant will scale as $l^{-(2\alpha+\delta)}$. Since the elastic modulus is obtained by multiplying the force constant by l^{2-d} , we find that for a single chain $\tilde{\tau}_s = d - 2 + 2\alpha + \delta$. Clearly the elastic modulus of the entire structure is larger than or equal to the elastic modulus of a single branch, and therefore $\tilde{\tau}_s$ is an upper bound on the critical exponent $\tilde{\tau}$ of DLA. Since DLA has no loops larger than several lattice constants it can be shown (Witten and Kantor 1984) that under certain homogeneity assumptions this is not only a bound but the actual value of $\tilde{\tau}$. Thus for $d=2$ we can obtain the values of $\tilde{\tau}_c$ and $\tilde{\tau}_\mu$ by substituting the correct values of α and δ in the relation $\tilde{\tau} = 2\alpha + \delta$. Meakin *et al* (1984) have found the exponent δ to be indistinguishable from 1. To evaluate $\tilde{\tau}_\mu$ in this way we must find the radius of gyration in the y direction of a typical branch (see figure 1). Obviously this is simply proportional to l , and therefore $\alpha_\mu = 1$ and $\tilde{\tau}_\mu = 3$. The situation is less clear with respect to $\tilde{\tau}_c$: because the total length of a branch is apparently proportional to l ($\delta = 1$), it is conceivable (and is indeed suggested by figure 1) that some of the spanning branches have a radius of gyration in the x direction which grows more slowly than l (i.e. $\alpha_c < 1$). In that case, $\tilde{\tau}_c$ is determined by the branches with the *smallest* radii of gyration, rather than by the typical branches, and we would get $\tilde{\tau}_c < \tilde{\tau}_\mu$. Thus, while we cannot estimate the value of $\tilde{\tau}_c$ from purely geometrical considerations we may expect it to be smaller than 3.

We calculated the effective moduli, c and μ , for computer simulated strips of different widths l . For given l we used the part of the aggregate with $1 \leq y \leq l$. Figure 2 depicts the power law dependence of the moduli on l . To obtain the results shown

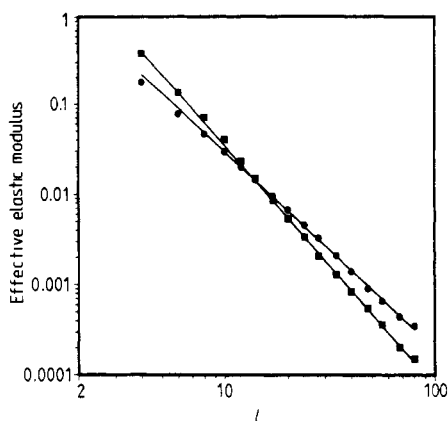


Figure 2. Double logarithmic plot showing the dependence of the shear modulus (multiplied by 10) μ (■) and the stretching modulus c (●) on the width of the strip l .

there we used such values of the microscopic force constants which produced $\kappa_1 = 100$ and $\mu_1 = 1$. In this case $k/m = 1194$. A decrease of this ratio by almost two orders of magnitude did not cause any significant effect, since the asymptotic slope does not depend on k (cf Kantor and Webman 1984). The large value of k/m was chosen to reduce to a minimum the crossover effects. The estimated errors in the value of each point on figure 2 increase from 3% for small l to 10% for large l . (They are smaller than the sizes of the symbols depicting the points.) Both curves have a detectable curvature for small widths of the strip. Slopes of these curves are equal to $\tilde{\tau}$. We estimate $\tilde{\tau}_\mu = 2.6 \pm 0.2$ and $\tilde{\tau}_c = 2.2 \pm 0.2$, where the error bars represent our subjective assessment of a possible systematic error due to the short linear range of these graphs. A further increase in the accuracy of these values would require the use of considerably wider and longer strips, which is at present beyond our computer possibilities. However, it seems that the inequality $\tilde{\tau}_c < \tilde{\tau}_\mu$ is well established.

In this work we calculated the critical scaling indices of the elastic moduli of DLA, and showed that their values depend on the direction of the applied deformation. It would be interesting and useful to perform similar three-dimensional calculations. However, we can expect to get the same or very close values of $\tilde{\tau} - d$ in any space dimensionality. The appearance of two different $\tilde{\tau}$'s implies the existence of two different types of vibrational states with a different dependence of the density of states on the frequency. Finally, it would be interesting to know whether the value of $\tilde{\tau}_c$ can be determined from purely geometrical considerations.

References

- Bergman D J 1985 *Phys. Rev. B* **31** 1696
- Brady R M and Ball R 1984 *Nature* **309** 225
- Derrida B and Vannimenus J 1982 *J. Phys. A: Math. Gen.* **15** L557
- Elam W T, Wolf S A, Sprague J, Gubser D U, Van Vecht D, Barz G L Jr and Meakin P 1985 *Phys. Rev. Lett.* **54** 701
- Family F and Coniglio A 1984 *J. Phys. A: Math. Gen.* **17** L285
- Kantor Y and Webman I 1984 *Phys. Rev. Lett.* **52** 1891
- Kantor Y and Witten T A 1984 *J. Physique Lett.* **45** L675

- Mandelbrot B B 1982 *Fractal Geometry of Nature* (San Francisco: Freeman)
- Matsushita M, Sano M, Hayakawa Y, Honjo H and Sawada Y 1984 *Phys. Rev. Lett.* **53** 286
- Meakin P 1983a *Phys. Rev. A* **27** 1495
- 1983b *Phys. Rev. A* **27** 2616
- Meakin P, Majid I, Havlin S and Stanley H E 1984 *J. Phys. A: Math Gen.* **17** L975
- Meakin P and Vicsek T 1985 *Preprint*
- Nittman J, Daccord G and Stanley H E 1985 *Nature* **314** 141
- Rácz Z and Vicsek T 1983 *Phys. Rev. Lett.* **51** 2382
- Webman I and Grest G 1985 *Phys. Rev. B* **31** 1689
- Witten T A and Kantor Y 1984 *Phys. Rev. B* **30** 4093
- Witten T A and Sander L M 1981 *Phys. Rev. Lett.* **47** 1400
- 1983 *Phys. Rev. B* **27** 5686