On Biharmonic Fractals Displaying a Structural Transition

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A new class of fractal structures displaying a structural transition on growing is studied by considering the morphology selection mechanism under the biharmonic field $\nabla^2(\nabla^2 u) = 0$ as recently proposed by the authors [Phys. Rev. E **47,** 476 (1993)]. By relating the growth probability for each site to the local ("potential") field as $(\nabla^2 u)^\eta$, the effects of the surrounding medium and of geometrical constraints for the seed particles are numerically calculated and discussed. A theoretical estimation of the transition point is given anew by solving the biharmonic equation with the boundary conditions used in simulations.

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1. Introduction

Fractal pattern formation has become a mainstream topic in the last decade. Far-from-equilibrium structures, like flakes, soot or dust in sedimentation flocculation and aggregation, are examples of natural entities with an inherent nontrivial scaling symmetry. Great progress has been made in understanding this kind of patterns, mainly due to the introduction of the concept of fractality in conjunction with sophisticated computer simulations of simple but nontrivial growth models.

In particular, much attention has been focused on the fractal growth within the Laplacian field, such as the diffusion-limited aggregation (DLA) and the dielectrical breakdown model (DBM). Their implementations give rise to a variety of morphologies which have been linked to patterns arising in several nonequilibrium growth processes (see, e.g. [1, 2]).

However, it has been recently discussed that there exists another important field, which can also support the fractal growth with a rich variety of structural behaviour. One example is the Poisson field $\nabla^2\phi = \lambda^2\phi$ [3–5]. In this case, such a field generates complex fractal patterns displaying a structural transition on growing named "transition from dense to multi-branched growth" by the authors of [3].

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On the other hand, we have recently introduced in [6, 7] an alternative model from which one can also derive a fractal structure displaying a peculiar structural transition, the so-termed biharmonic model. From a physical viewpoint, the biharmonic equation is relevant to describe the deflection of a thin plate subjected to uniform loading over its surface with fixed edges, the steady slow two-dimensional motion of a viscous fluid, or the vibration modes in the acoustics of drums.

In [6, 7] we have proved that the biharmonic equation

$$\nabla^2(\nabla^2 u) = 0 \tag{1}$$

drives a structural transition due to the coupling between displacements u (at sites i, j), that strongly differ from the simpler Laplacian model [8] or the Poisson growth [3]. Within this biharmonic model, however, the structural transition appears when the velocity on the growing surface presents a minimum, as also occurs within the Poisson growth (assumed to be proportional to an equivalent "electric" field at the surface of the aggregate [3]).

It is the purpose of this paper to analyse in more details biharmonic fractals within the domain of physically interesting parameters. Herein we shall follow our previous ideas to analyze anew the effects of the sourrounding medium and of geometrical constraints for the seed particles on biharmonic fractal growth.

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We shall also give a new analytical estimation of the transition point.

The motivation for this work was twofold. On the one hand little numerical and theoretical work exists about fractal surfaces that become complex when structural transitions are generated on growing. Thus a study as the one at hand can help to uncover the physics behind these phenomena. On the other hand, despite the fact that the mechanisms involved on such processes can be quite different, as for example during bacterial colony [9] and electrochemical deposition [10] experiments, the measured fractal patterns might be seen as belonging to a similar class of complex structures. Hence different theoretical viewpoints, giving apparently similar results, are necessary to get deeper insight into such an intriguing problem.

2. Biharmonic Fractals and Local Growth Probability

The inclusion of second and higher nearest neighbour bond shells in the present numerical simulations, following the discrete form of (1) on the (i, j) lattice site, yields an expression involving values of u at 13 mesh points:

$$\begin{aligned} u_{i-2,j} &+ 2u_{i-1,j-1} - 8u_{i-1,j} + 2u_{i-1,j+1} \\ &+ u_{i,j-2} - 8u_{i,j-1} + 20u_{i,j} - 8u_{i,j+1} \\ &+ u_{i,j+2} + 2u_{i+1,j-1} - 8u_{i+1,j} + 2u_{i+1,j+1} \\ &+ u_{i+2,j} = 0 . \end{aligned}$$

Using this discretization, the calculations become more involved than for Laplace [8] or Poisson [3] growth because of the coupling between displacements u. However, the accuracy of the solution of (2) can similarly be improved by looking at the convergence of the iterative solution using the well-known Gauss-Seidel method.

Equation (1) requires modification when applied at mesh points that are adjacent to a boundary, since one (at the edge) or two (near the corners) of the values needed are at sites outside the lattice. This modification is made by introducing a fictitious mesh point at (i, L) outside the planar lattice in the y-direction, where the value of u is given by the derivative boundary condition along one edge boundary:

$$u_{i,\,L+1} = u_{i,\,L-1} + 2h \left.\frac{\partial u}{\partial y}\right|_{i,\,L} . \tag{3}$$

Here $h\ (=h_x=h_y)$ is the mesh size which we set equal to unity for simplicity. For planar geometry, we evaluate (3) as

$$\left.\frac{\partial u}{\partial y}\right|_{i,\,L} \approx \frac{3(u^0 - u^i)}{L} \tag{4}$$

for all i-columns. This expression is obtained after taking the limit $l/L \ll 1$ in the solution of a 1 D biharmonic equation. For circular geometry we treat the boundary conditions similarly to Laplacian growth [8], i.e., all the lattice sites outside a circle of radius r are set equal to u^0, hence, we approximate

$$\left.\frac{\partial u}{\partial y}\right|_{y=L} \approx 0 \tag{5}$$

in the absence of an external field.

In this way, throughout the present calculations we use lattice sites enclosed within a circle of (normalized) radius $L = \sqrt{i^2 + -j^2} = 100$ such that u^0 and u^i are unity and zero at the outer circular boundary and the inner growing biharmonic aggregate, respectively. Seed particles are placed either centered or distributed under different geometrical constraints. The procedure for growing fractals then follows standard techniques [8], till solutions of the discretization of (1) converge to a desidered accuracy (of the order 3×10^{-3} or smaller). After adopting a growth probability law, aggregates stochastically grow under the given relation between the growth probability P (at the grid site (i, j)) and u.

To mimic effects of the surrounding medium on biharmonic fractal growth we follow the η (or dielectric breakdown) model [8] and assume

$$P_{ij} = \frac{|\nabla^2 u_{i,j}|^\eta}{\sum |\nabla^2 u_{i,j}|^\eta} , \tag{6}$$

where the sum runs over nearest neighbor sites to a biharmonic cluster. This implies that P_{ij} is proportional to the local ("potential") field with $\eta \geq 0$.

3. Results and Discussion

In this work we extend our previous simulations [6, 7] to values of $\eta \neq 1$. Figure 1 shows our numerical results by using several values of η, namely $\eta = 3$ with 383 particles, $\eta = 2$ with 996 particles, $\eta = 1$ with 2293 particles, $\eta = 0.75$ with 3332 particles, $\eta = 0.5$ with 4000 particles added to the biharmonic aggregates.

The CPU time required to grow the denser clusters was nearly 12 hours on a Convex C210 supercomputer machine.

For the sake of simplicity, the derivative boundary condition required along the r-direction has been set equal to zero. As also done in [6, 7], we fixed $u^i = 0$ and rescaled (the equivalent "potential") $\phi^0 \equiv \nabla^2 u|_{y=L}$ such that $u^0 = 1$. This means having the relation

$$\nabla^2 u|_{y=L} \approx 6/L^2 . \quad (7)$$

Similarly to Laplacian growth [8, 11], the influence of ramified biharmonic fractals on the growth probability for each lattice site depends on the type of pattern generated (i.e., more or less dense). On decreasing the value of η, we also find a transition from *dendritic-to-compact* growth such that the inner region of the aggregates becomes denser. If $\eta \to 0$, the growth probability becomes purely random and independent of the biharmonic field (as a Eden-like model). But, as a key difference, in our model there is a transition from dense to multibranched growth due to the biharmonic law of growth, as can be seen in all cases illustrated in Fig. 1, except for the dendritic patterns. Clearly, in the limit $\eta \to \infty$ this phenomenon can no longer be named "dense-to-multibranched transition". It is instead a "*transition from slow to faster growth*", in the sense that one end of the needle-like structure presents greater growth probability than the other. Such structures become dendritic below above their transition points, which we shall estimate next.

Let us first calculate the fractal dimension d_f of the biharmonic patterns in Fig 1 via the standard box counting method, i.e by counting the number of particles $N(r)$ inside an increasing radius r (around a seed particle) even if it falls beyond the transition point. We then plot this sum as a function of r in a double logarithm plot as shown in Figure 2. Over a decade, we obtain straight lines with slopes between unity and the space dimension as indicated. In the lower r-region, i.e. below the transition points, d_f's for clusters with $\eta = 1$ approach the value of Laplacian growth (i.e. $d_f \approx 1.7$), whereas for $\eta \to 0$ we get the d_f value of the Eden model (i.e., $d_2 \approx 2$). For $\eta > 1$ we obtain the fractal dimension typical of denditric growth ($d_f \approx 1$).

Figure 2 not only illustrates the fractal nature of our biharmonic patterns, but it also helps us to locate approximately the transition points as a function of η, at least for $\eta \leq 1$. This quantification is justified because of the lack of a simple theoretical approach in the case $\eta \neq 1$. Clearly the changes of slope in the

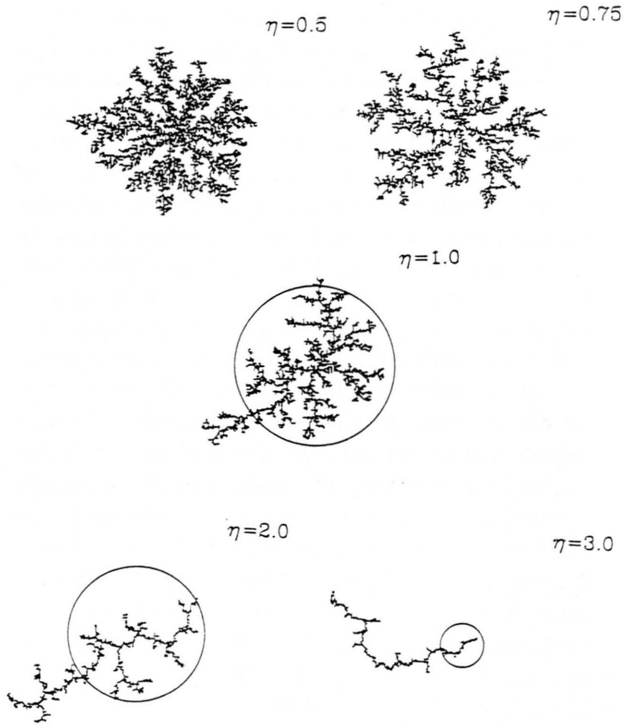

Fig. 1. Biharmonic fractals in circular geometry for different values of η. Circles approximately indicate the respective transition points.

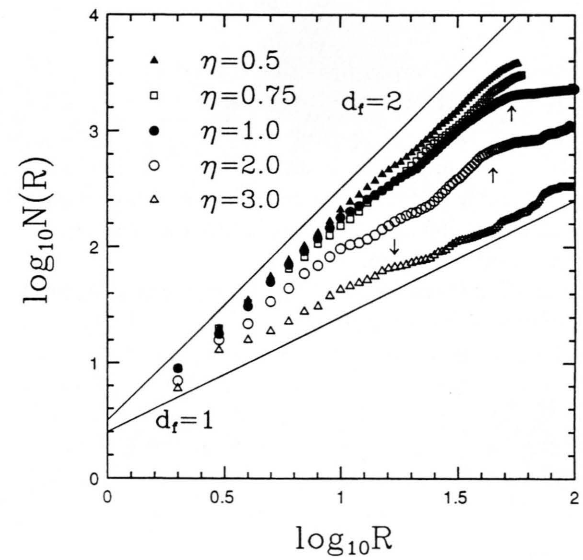

Fig. 2. Fractal nature of the biharmonic patterns in Figure 1. Arrows indicate transition points.

large-r regime, that are indicated by arrows in Fig. 2 (below the limit of $L/2$), correspond to the transitions enclosed by circles in Figure 1. On decreasing $\eta < 1$, we find that the transition points shifts towards higher values of the distance from the seed particles. However, if $\eta \to 0$, large-scale simulations are necessary to reach the transition point and obtain the required precision for the convergence of solutions of (1). In the case of generating needle-like structures with $\eta > 1$ the clusters grow relatively faster, so we locate the transition point from the (rather short) distance from the seed to the cluster's end, which grows more slowly.

In analyzing the above transition we are also interested in inferring the effects of geometrical constraints (or boundary conditions) for the seed particles. This can be done by fixing the value of η and adopting different forms for the distribution of seed particles. In Fig. 3 we show biharmonic fractals with $\eta = 1$ which grow under two different geometries for the seed particles, namely circular and linear. In both cases we have used a simulation box of size 100 × 100 to grow a cluster of about 1450 particles having a circular seed, and 900 having a linear seed. To avoid approaching the boundary of the simulation box, these geometrical constraints limit to a domain smaller than 1/3 of the system size. From this figure it can be seen that the so-formed biharmonic structures present a transition at about 0.6 (indicated by arrows). But, the difference with respect to biharmonic fractals generated from a single-point substrate is in the final pattern obtained, that is still fractal, and not on locating the transition. From these results, under both circular and linear constraints, we proved that the transition still survives independently of the chosen seed configuration.

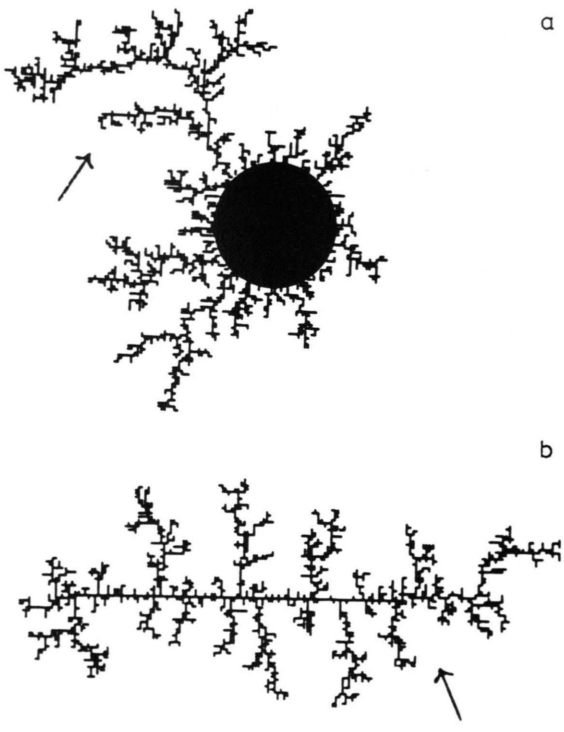

Fig. 3. Biharmonic fractals with $\eta = 1$ under (a) circular and (b) planar geometries for the seed particles.

In addition to this we have also done runs for $\eta = 1$, either for the big lattice size with $L = 120$ and 200, or for the smaller lattice size with $L = 60$. We have found that in all cases there exists a transition at around 60% of the system size, as theoretically predicted by solving analytically the biharmonic equation in cylindrical coordinates such that $z = 0$ for all polar angles θ.

Let us focus now on a possible theoretical description for the transition point r_l at $\eta = 1$. A first crude attempt to evaluate r_l was made in [6], however these calculations need to be revised. A more complete analysis is given next.

The biharmonic equation (1) in cylindrical coordinates becomes

$$\frac{1}{r^2}\left(\frac{\partial u}{\partial r}\right) - \frac{1}{r}\left(\frac{\partial^2 u}{\partial r^2}\right) + 2\left(\frac{\partial^3 u}{\partial r^3}\right) + r\left(\frac{\partial^4 u}{\partial r^4}\right) = 0\,, \quad (8)$$

whose solution far from the origin is

$$u(r) = A + Br^2 + C\,\ln(r/L) + Dr^2\,\ln(r/L)\,. \quad (9)$$

In the above A, B, C, and D are four constants characteristic of a differential equation of order four, and r has been normalized with respect to the system size L.

Another unknown coefficient of our problem is the transition point r_l, which together to A, B, C, and D can in principle be specified in terms of L provided one establishes five different conditions for u of (9). To this end we adopt the four boundary conditions used in the present simulations, namely, (i) $u(r_l) = u^i \equiv 0$ at $r = r_l$, (ii) $u(L) = u^0 \equiv 1$ at $r = L$, in conjunction with (iii) (5) and (iv) (7).

To specify the required fifth boundary condition it is natural to relate this to a property displayed by the biharmonic (and/or Poisson) fractals. The most important of them concerns the growth velocity at the growing surface. As mentioned in the introduction, we have previously found that the structural transition occurs when this velocity (assumed to be proportional to an equivalent "electric" field at the surface of the aggregate) presents a (non-zero) minimum. Let us an-

Table.

Boundary condition	$\delta=0$	Unique solution	Simulations fit $r_l \approx 0.6$
$\left.\frac{\partial^2 u}{\partial r^2}\right\|_{r_l} \equiv \frac{\delta}{L^2}$	n.s.	$\delta = -56.890$; $r_l = 0.433$	$\delta = -69.109$
$\nabla^2 u\|_{r_l} \equiv \frac{\delta}{L^2}$	n.s.	$\delta = -32.751$; $r_l = 0.275$	$\delta = -52.715$
$\left.\frac{\partial}{\partial r}\left(\frac{\partial^2 u}{\partial r^2}\right)\right\|_{r_l} \equiv \frac{\partial}{L^3}$	n.s.	$\delta = 286.999$; $r_l = 0.485$	$\delta = 334.074$
$\nabla(\nabla^2 u)\|_{r_l} \equiv \frac{\delta}{L^3}$	n.s.	$\delta = 107.087$; $r_l = 0.325$	$\delta = 191.569$

alyze this fact from a theoretical point of view as indicated below.

In the Table, we consider four possible ways to relate the growth velocity at the circular surface δ, to the potential or the field (i.e., D'Arcy's like law). If δ vanishes we found that there is no solution (n.s.) for the set of equations at hand, independently of taking any of the four boundary conditions described in the Table. Nicely, this simple prediction is in accord with our previous numerical simulations regarding the non-zero value for the growth velocity at r_l. However, within the present theoretical framework this value does not correspond to a minimum. On the other hand, the predictions for a unique r_l-value, obtained from the solutions (9) of the biharmonic equation in cylindrical coordinates, slightly disagree with the simulations. From the Table it can be seen that r_l changes between 0.275 and 0.4865. After a little algebra, we have found that the structural transition can occur at about 60% of the system size only if the parameter δ is allowed to vary (increasing or decreasing depending on the boundary condition adopted). Because of this, we conclude that the location of the biharmonic structural transition point is still an open question.

4. Concluding Remarks

We have shown that by tuning $\eta \to 0$, the structural transition corrresponds to a "dense-to-multibranched transition" whereas for $\eta \to \infty$ we get a "transition from slow to faster growth". From the numerical simulations we have found that the transition occurs at about 60% distant from the center only if $\eta = 1$. Theoretically, we have seen that the predictions for a unique r_l value, obtained from the solutions (9) of the biharmonic equation in cylindrical coordinates, slightly disagreed with simulations.

On decreasing η from infinity to zero, biharmonic fractals become denser than for Laplacian growth. Their respective transition points move outward when keeping L fixed. For large η, the needle-like structures grow faster at one end and remain essentially denditric. In this respect, we add that similar conclusions apply for biharmonic growth in planar geometry (results not shown). We have also shown that the transition point is independent of the configuration adopted for the seed particles. Within the biharmonic approach, the aggregate is fractal before the transition point r_l with the fractal dimension approaching the standard DLA or DBM aggregates.

To complete this study, we have also checked our results against some smaller values for the convergence of the iterations for the discretized biharmonic equation. For the smaller value we used, the transition point slightly shifts towards values smaller than 0.6, i.e. the inner limit of the fractal aggregate moves inwards.

The study in this paper is a logical extension of our previous work, and is intended to contribute to the understanding of the complex pattern formation under the biharmonic field which is obviously different from the Laplacian and Poisson fields. In fact, the structural transition modelled in the present systems is due to the coupling between the u-displacements (cf. (2)). This is a somewhat different cause for driving this phenomenon than the screening effect as suggested in [3].

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