Needle crystal formation in two dimensions

1986 J. Phys. A: Math. Gen. 19 L1109

(http://iopscience.iop.org/0305-4470/19/17/011)

J. Phys. A: Math. Gen. 19 (1986) L1109–L1115. Printed in Great Britain

LETTER TO THE EDITOR

Needle crystal formation in two dimensions

J Szép† and E Lugosi‡

† Department of Solid State Physics, Eötvös University, Muzeum krt 6–8, H-1088, Budapest, Hungary

‡ Mathematical and Physical Journal for High School Students, PO Box 566, H-1374, Budapest, Hungary

Received 15 May 1986

Abstracts. A simple model (based on conformal mapping) is constructed to simulate two-dimensional growth of needle crystals growing out regularly from a common point. The resulting patterns are very similar to those which were obtained by other methods. The radius of gyration exponent β is measured and found to be in the range 0.58–0.65, independent of the number of needles (n). It is shown that for large patterns, β asymptotically approaches a value of $\frac{2}{3}$. To compare our patterns with the DLA aggregates, the average slope (α) was measured for the density-density correlation function plotted logarithmically ($\log r \to \log C(r)$). The relation between α and β, which is characteristic of DLA fractal aggregates, is satisfied only in the case $n = 8$.

In recent years, pattern formation in such diffusion-controlled processes as solidification or viscous fingering, has attracted great interest. Growth has been investigated by various methods, e.g. the boundary layer model (Ben-Jacob *et al* 1984, Karma and Kotliar 1985), the numerical solution of the Laplace equation (Chen and Wilkinson 1985), through the use of conformal mapping (De Gregoria and Schwartz 1985) and the Monte Carlo (MC) method.

The fundamental MC method, the diffusion-limited aggregation (DLA) model, was introduced by Witten and Sander (1981). The result of this model is a fractal object (see Mandlebrot 1982) in which the fluctuations, originated in the MC method, have an important role. To damp the fluctuations by averaging, another MC method was introduced by Tang (1985), Szép *et al* (1985) and Kertész *et al* (1986). Kertész and Vicsek (1986) then included the averaging in the DLA model, and at large averaging they obtained regular needle crystals.

Let us take the following equations which describe the growth of a pattern:

$$\nabla^2 U = 0 \tag{1a}$$

$$(\partial\Gamma/\partial t)_n = D(\nabla U)_n \tag{1b}$$

$$U|_\Gamma = 0 \tag{1c}$$

where Γ represents any point on the boundary, and n its normal direction.

U can correspond to several physical quantities like the temperature or concentration in the solidification (see Langer 1980), the pressure in the Hele–Shaw experiment (Kadanoff 1985) or the probability of finding the moving particle in DLA (Witten and Sander 1981). D corresponds to the diffusion constant. Equation ($1c$) represents the vanishing surface tension case.

0305-4470/86/171109+07\$02.50

We also have another boundary condition: fixing the origin at the seed of the pattern

$$\frac{U(r)}{\log|r|} \xrightarrow[|r|\to\infty]{} C \tag{1d}$$

where C is a constant.

Our aim is to construct a relatively simple model to determine the shape of needle crystals (NC). Langer (1986) has shown that the direction of the NC does not change during growth in the presence of a slight anisotropy in the surface tension. Here we present a simple approximative scheme where we neglect the surface tension; anisotropy is involved only in the starting configuration, and it is assumed that the direction of the needle does not change. Our approach is based on the solution of the Laplace equation for idealised needles.

The growth velocity of the tip is much greater than the growth velocity of the side surface. During growth, the width/length ratio for the needles is decreasing. The slight width of the needles has only a small effect on the growth. The main assumption in our model is to disregard this effect.

In the calculation of grad U, the width of the needle is neglected. This allows easy evaluation of the gradient at the side of the needle. However, at the tip of the needle, the gradient has divergence. For this reason the gradient is determined by finite differences. Let our local coordinate system be chosen in such a way that the origin is at the location of the seed, the coordinate x is in the direction of the needle and y is perpendicular to it. At the tip of this needle equation $(1b)$ becomes

$$\frac{\mathrm{d}s}{\mathrm{d}t} = D\frac{U(s+\Delta_1, 0)}{\Delta_1} \tag{2}$$

where s is the length of the needle.

In addition, equation $(1b)$ for the side surface of the NC becomes

$$\frac{\partial W(x, s)}{\partial t} = D\frac{U(x, \Delta_2)}{\Delta_2} \tag{3}$$

where W denotes the half width of the needle of length s at a distance x from the origin, and Δ_1, Δ_2 are fixed small values. The above two equations are the basic assumption of our model.

It can be seen that the tip of an NC growing in our model, according to equations (2) and (3), corresponds to the tip of a real parabolic needle crystal (which is the two-dimensional case of the Ivantsov model) with tip radius $\Delta_1/2$ (i.e. $W = (\Delta_1(s-x))^{1/2}$ if $s - x \ll s$).

Furthermore, DLA is a discrete model, where $\Delta_1 = \Delta_2 = 1$ lattice unit.

In the following, we examine the growth of NC placed in a regular shape. It is easy to solve the Laplace equation in the case of a pattern consisting of rods of zero width placed regularly as an n-fold. The conformal map

$$f(z) = s^{-1}[z^{n/2} + (z^n - s^n)^{1/2}]^{2/n} \tag{4}$$

maps the pattern described above into the circle of unit radius. Taking $(1c)$ and $(1d)$ into account, the solution of $(1a)$ is

$$U(x, y) = C\log|f(x+\mathrm{i}y)|. \tag{5}$$

Equations (2) and (3), using (5), are easily solved numerically by computer. Results in the present letter were obtained by choosing $\Delta_1 = \Delta_2 = C = D = 1$. Thus, we assume that the tip radius does not change during the growth. The patterns were grown from the $s = 1$, $W \equiv 0$ initial state. Figure 1 shows NC calculated by this method for $n = 6$ and $s = 740$.

Figure 2 shows the width profile $W(x, 740)$. As n increases the parts near the origin are more screened. Therefore, the distance m between the origin and the point of

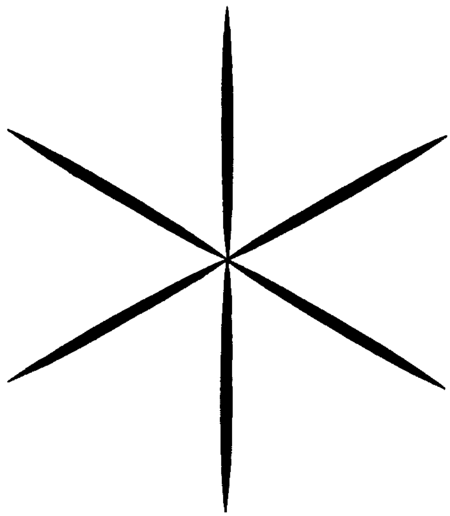

Figure 1. Regular needle crystals grown by our method. The radius of the pattern is 740 units, while the tip radius is 0.5 units.

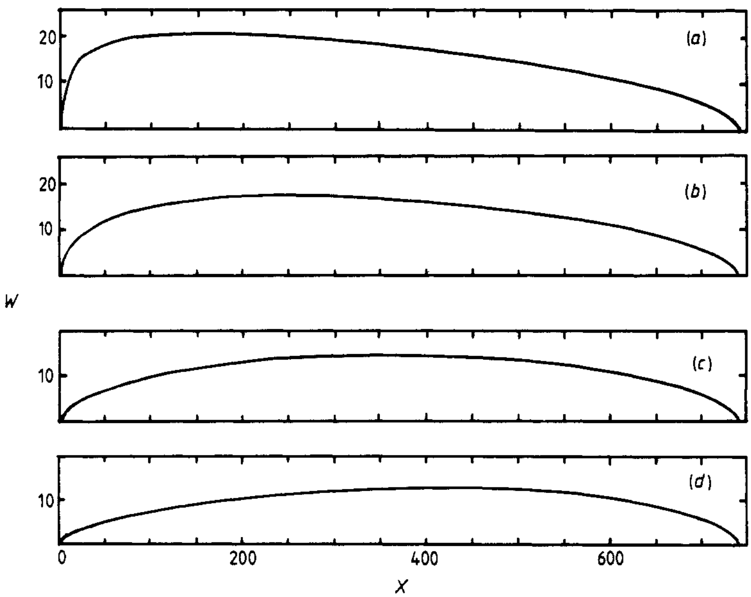

Figure 2. Half-width profiles of needle crystals; n denotes the number of needles growing from the origin; (a) $n = 3$, (b) $n = 4$, (c) $n = 6$, (d) $n = 8$.

maximal width increases: $m_{n=3} = 0.22\ s$, $m_{n=4} = 0.33\ s$, $m_{n=6} = 0.48\ s$, $m_{n=8} = 0.56\ s$. In the case of $n = 4$, the point of maximal width is a distance $s/3$ from the origin. For $n = 6$ the width profile is quasi-symmetrical. These shapes are similar to the averaged DLA patterns grown by Kertész and Vicsek (1986) ($n = 4$, $n = 6$), to the experimental results of Ben-Jacob *et al* (1985) ($n = 6$) and to the experimental and theoretical results of Chen and Wilkinson (1985) ($n = 4$). The stability of the tip was due to the anisotropy of a grid in these cases.

Figure 3 shows in a log-log plot the radius of gyration (root-mean-square distance from origin), calculated during the growth, as a function of the area of the pattern. The slopes of the curves are almost independent of n, and their values are

$$\beta_{s=20} = 0.581 \pm 3\% \qquad \beta_{s=50} = 0.628 \pm 1.5\% \qquad \beta_{s=200} = 0.650 \pm 1\%.$$

In the following we shall see that exponent β asymptotically approaches the value of $\frac{2}{3}$. It is easy to see that, in any direction from the tip, the value of U is proportional to the square root of the distance from the tip (provided the distance is small). Likewise, near the line $U = 0$, U is proportional to the distance from the line. Therefore, on the basis of (2)-(5)

$$\mathrm{d}s/\mathrm{d}t = g_0/\sqrt{s} \tag{6}$$

and

$$\partial W(x, s)/\partial t = s^{-1} g(x/s) \tag{7}$$

hold asymptotically when s is large enough. Furthermore, g_0 is a constant and the function $g(x)(0 < x < 1)$ is proportional to the gradient of U at the side surface of an NC of unit length. Using these equations we obtain

$$\frac{\partial W(\lambda x, \lambda s)}{\partial t} = \lambda^{1/2} \frac{\partial W(x, s)}{\partial t} \qquad (\lambda > 0)$$

from which

$$W(\lambda x, \lambda s) = \lambda^{1/2} W(x, s) \tag{8}$$

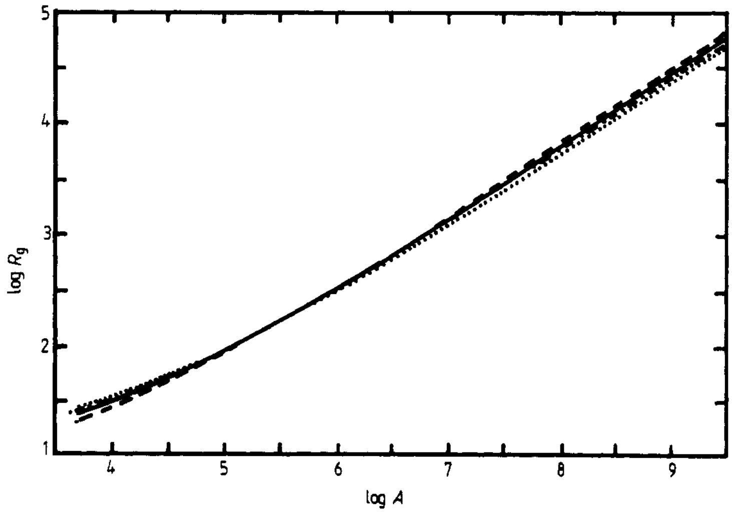

Figure 3. Log-log plot of the radius of gyration function. The slope is in the range 0.58-0.65; curves are $n = 3$ (- - - -), $n = 4$ (——), $n = 6$ (·—·—·) and $n = 8$ (. . . . . . .).

follows; i.e. W is a homogeneous function of one half order. This shows that we have affine self-similarity: during their growth the NC do not change shape; they only decrease in width/length ratio. This was actually seen in a graphical display of a computer-simulated NC growth. Denoting the area of an NC of length s by $A(s)$, the radius of gyration by $R_g(s)$ and using equation (8), it follows that

$$R_g(s) = (R_g(s_0)/A^{2/3}(s_0))A^{2/3}(s)$$

where s_0 is a constant. We arrive at the result that asymptotically $\beta = \frac{2}{3}$. This is in agreement with the theoretical result of Turkevich and Scher (1985) derived for the two-dimensional DLA model with sharp tips, and the numerical results of Nittman and Stanley (1986).

Figure 4 shows logarithmically the density–density correlation function. $C(r)$ is the average value of $A^{-1}\iint \rho(\boldsymbol{r}')\rho(\boldsymbol{r}+\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}'$, when $|\boldsymbol{r}| = r$. The density $\rho(\boldsymbol{r})$ is defined to be 1 inside the NC and 0 outside. For us, only the $2W < r \ll 740$ (i.e. $3 < \log r < 6$) part of the curve is of importance. As n increases the average slope increases and the dependence of r is stronger. The average slopes, obtained by the least-squares method, for the $3 < \log r < 6$ part of the curves are

$$\alpha_{n=3} = -0.98 \qquad \alpha_{n=4} = -0.83 \qquad \alpha_{n=6} = -0.66 \qquad \alpha_{n=8} = -0.51.$$

For the fractal patterns grown by the DLA model, the equation $D = 1/\beta = d + \alpha$ is satisfied (D is the fractal dimensionality, d the Euclidean dimensionality and, in this case, $d = 2$). For the NC patterns growing by our model, the value of α depends strongly on n while the value of β does not. The equation $1/\beta = 2 + \alpha$, characteristic of fractals, comes true in our model for $n = 8$ only. The number of main branches of patterns growing by the standard DLA model cannot be counted because of its random characteristic. However, the number of main branches can be defined as follows:

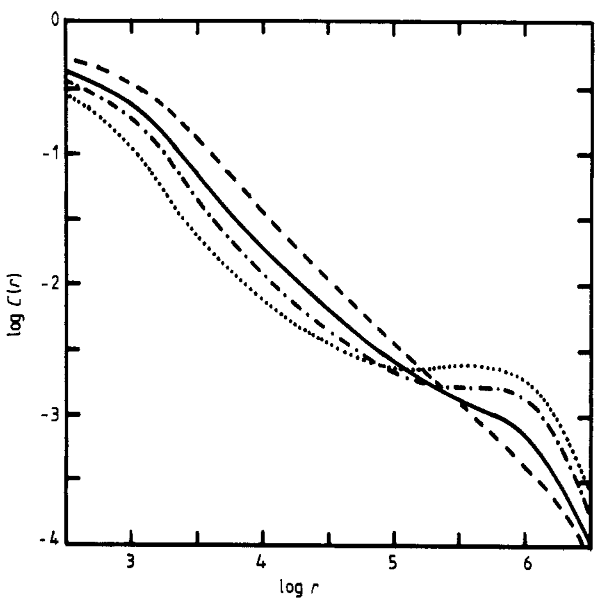

Figure 4. Log-log plot of the density-density correlation function of needle crystals (as in figure 1) for various numbers of needles; curves are $n=3$ (- - - -), $n=4$ (——), $n=6$(·—·—·) and $n=8$ (· · · · ·).

$n = \Pi/\Theta_{\min}$, where $\Theta_{\min}$ is the angle for which the tangential correlation function $C(\Theta)$, introduced by Meakin and Vicsek (1985), has minimum value. In the DLA model, $\Theta_{\min} = 0.35 \pm 0.04$, hence $n = 9 \pm 1$ for off-lattice aggregates. This is based on a measurement of $C(\Theta)$ by Meakin and Vicsek (1985). It is interesting that this value is essentially the same we obtain in our model when $1/\beta \simeq 2 + \alpha$.

Figure 5 shows logarithmically the average density as function of the distance from the origin: $\bar{\rho}(r) = nW(r, 740)/r\Pi$.

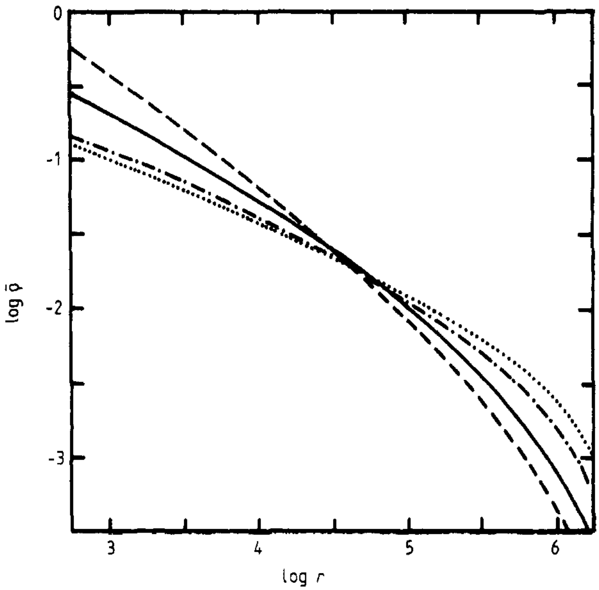

Figure 5. Log-log plot of the average density as a function of the distance from the origin. Curves are $n = 3$ (- - - -), $n = 4$ (——), $n = 6$ (·—·—·) and $n = 8$ (· · · · ·).

We introduced a relatively simple model to describe the growth of NC growing regularly from a common point. Such patterns are produced by the averaged DLA model (Kertész and Vicsek 1986) by solving the Laplace equation by Gauss-Seidel iteration (Chen and Wilkinson 1985), and by experiment (Chen and Wilkinson 1985, Ben-Jacob *et al* 1985). The patterns grown by our model are in good agreement with the previous ones.

These patterns are not fractals. Our equations describing the growth are the same as those for the case when, as the result of fluctuations, the growing patterns are fractals (see Kertész and Vicsek 1986). Our model can also be taken to be the large averaging limit of the DLA model on a grid.

The authors thank G Tichy, J Kertész and T Vicsek for useful comments on the manuscript.

References

Ben-Jacob E, Godbey R, Goldenfeld N D, Koplik J, Levine H, Mueller T and Sander L M 1985 *Phys. Rev. Lett.* **55** 1315

Ben-Jacob E, Goldenfeld N, Langer J S and Schön G 1984 *Phys. Rev.* A **29** 330

Chen J D and Wilkinson D 1985 *Phys. Rev. Lett.* **55** 1892
De Gregoria A J and Schwartz L W 1985 *Phys. Fluids* **28** 2313
Kadanoff L P 1985 *J. Stat. Phys.* **39** 267
Karma A and Kotliar B G 1985 *Phys. Rev.* A **31** 3266
Kertész J, Szép J and Cserti J 1986 *On Growth and Form* ed H E Stanley and N Ostrowsky (Dordrecht: Martinus Nijhoff) p 249
Kertész J and Vicsek T 1986 *J. Phys. A: Math. Gen.* **19** L257
Langer J S 1980 *Rev. Mod. Phys.* **52** 1
—— 1986 *Phys. Rev.* A **33** 435
Mandelbrot B B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)
Meakin P and Vicsek T 1985 *Phys. Rev.* A **32** 685
Nittman J and Stanley H E 1986 *Nature* **321** 663
Szép J, Cserti J and Kertész J 1985 *J. Phys. A: Math. Gen.* **18** L413
Tang C 1985 *Phys. Rev.* A **31** 1977
Turkevich L A and Scher H 1985 *Phys. Rev. Lett.* **55** 1026
Witten T A And Sander L M 1981 *Phys. Rev. Lett.* **47** 1400