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LETTER TO THE EDITOR

Growing self-avoiding surfaces

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Abstract. Two growing self-avoiding surfaces are introduced as possible models of rapidly polymerising polymer membranes. Monte Carlo simulations indicate that diffusion-limited self-avoiding surfaces have fractal dimension $D = 2.35 \pm 0.05$, and so are in a different universality class than diffusion-limited aggregates. In contrast, Eden self-avoiding surfaces appear to be compact, just as the clusters are in the usual Eden model. Both growing surfaces have different fractal dimensions than previously considered models of self-avoiding surfaces in equilibrium.

The equilibrium properties of flexible polymer chains are now reasonably well understood (de Gennes 1979). In addition, there has been significant progress in studying the growth of polymer chains far from equilibrium (Debierre and Turban 1986, Bradley and Kung 1986, Meakin 1988). Recently, intense theoretical interest has centred on the equilibrium behaviour of flexible polymer membranes (Redner 1985, 1986, Glaus 1986, 1988, Kantor *et al* 1986, 1987). The membranes are treated as random self-avoiding surfaces in these studies. The process of polymerisation, if present at all, is taken to be so slow that it may be neglected on the timescale characterising the fluctuations of the membrane.

In this letter, we look at the opposite limit in which the process of polymerisation is much more rapid than the internal fluctuations of the surface. The membrane grows by the addition of new plaquettes to its perimeter. Structural relaxation and thermal fluctuations within the membrane are neglected, just as in diffusion-limited aggregation (DLA) (Witten and Sander 1981) or the Eden model (Eden 1961). We will present results of Monte Carlo simulations of diffusion-limited growing self-avoiding surfaces (DLSAS) and Eden growing self-avoiding surfaces (ESAS) on a simple cubic lattice. In both models the basic constituent of the growing surface is a plaquette, i.e. a unit square of the lattice. Each of the four free edges of a plaquette may stick only once, when it overlaps a free edge belonging to another plaquette. The surfaces are strictly self-avoiding because two plaquettes are not allowed to occupy the same face of the lattice and also because no more than two plaquettes are allowed to have a common edge.

Although thermal fluctuations are neglected in both the DLSAS and DLA, these problems differ in one important respect: in the DLSAS each bond of the lattice can have at most two occupied plaquettes adjacent to it. This condition ensures that the surface is locally two-dimensional, a constraint which we shall see is relevant. This work on the DLSAS is a natural extension of our previous work (Debierre and Turban

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1986, Bradley and Kung 1986) on the diffusion-limited self-avoiding walk (DLSAW) in which each site on the aggregate is constrained to have at most two neighbouring bonds, so the polymers formed are topologically linear. The local constraint is relevant in the DLSAW, as it is for the DLSAS. Surprisingly, the ESAS appears to be in the same universality class as the usual Eden model in three dimensions.

In the DLSAS a seed plaquette is initially placed on an arbitrary face of a simple cubic lattice and is held fixed there. A sphere Σ of radius R_0 is drawn about the seed. A diffusing plaquette is then released at a randomly chosen point on Σ. The plaquette diffuses until one of its edges sticks to an edge of the seed plaquette. A second plaquette is then released on Σ, and it diffuses until it adheres to the perimeter of the membrane. This process continues with the addition of a third plaquette, a fourth plaquette, and so on. Each time a new plaquette is added to the growing surface, the maximum distance from the seed to a plaquette in the membrane, $R_{\max}$, is recomputed. We took $R_0 = R_{\max} + 5$. If any plaquette wanders further than $2R_0$ away from the seed, it is discarded and another diffusing plaquette is released on Σ. Finally, the growth process is terminated when part of the surface reaches the lattice boundary.

We must still describe how the moving plaquette diffuses. At each Monte Carlo step, one of the four edges of the diffusing plaquette is randomly selected and the plaquette is rotated around this edge by $+\pi/2$ or $-\pi/2$ with equal probability. The move is rejected if it brings an edge of the moving plaquette onto a lattice bond which already has two adjacent plaquettes. This special type of diffusion ensures that the surface will grow indefinitely, because when a new plaquette sticks to the surface perimeter, the edge around which it has last rotated remains free for further sticking. The centre of mass of the plaquette diffuses on a lattice different from the underlying cubic lattice, so we have not attempted to increase the diffusion step when the plaquette is far from R_0. With these rules, the DLSAS should apply to the diffusion-limited growth of a polymer membrane in a dilute solution of monomers, provided that the characteristic diffusion time is much shorter than the time characterising the relaxational dynamics of the membranes.

It is clear that the local constraint alters the short-range structure of the aggregates in the DLSAS. A crossover to the same scaling behaviour as in DLA in three dimensions cannot be ruled out *a priori*; however our simulations give strong evidence against such a crossover. Figure 1 gives a log-log plot of the radius of gyration R_g of the surfaces as a function of the number of plaquettes N they contain, the data being averaged over 100 samples on a $101 \times 101 \times 101$ lattice. For large surfaces, $R_g \sim N^{1/D}$ and we find a fractal dimension $D = 2.35 \pm 0.05$, in contrast to the result $D = 2.5$ for DLA in three dimensions (Meakin 1983a, b).

An equilibrium model of self-avoiding surfaces with the same excluded-volume constraints that we impose here has recently been studied by the exact enumeration method (Redner 1985, 1986). It is believed to belong to the same universality class as lattice animals (Durhuus *et al* 1984, Glaus 1986) which have fractal dimension $D = 2$ in three dimensions (Parisi and Sourlas 1981). Kantor *et al* (1986, 1987) studied the equilibrium self-avoiding surface with fixed connectivity. Their Flory theory and Monte Carlo work both point to a fractal dimension $D = 2.5$. Our result $D = 2.35 \pm 0.05$ strongly suggests that the DLSAS is in a different universaltiy class than both these models of self-avoiding surfaces in equilibrium.

We have also simulated Eden growing self-avoiding surfaces (ESAS) with the same self-avoiding constraints as for DLSAS. At each step, a new plaquette is allowed to occupy with equal probability any active perimeter face, i.e. any empty face connected

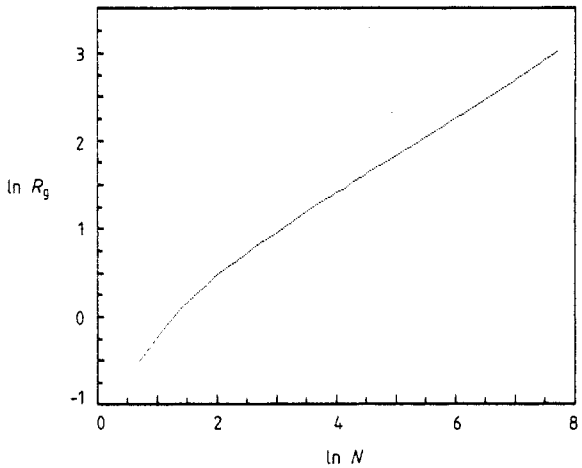

Figure 1. A log-log plot of the mean radius of gyration R_g against the size N, for the diffusion-limited self-avoiding surfaces. The values have been averaged over 100 samples of 2250 plaquettes on a $101 \times 101 \times 101$ cubic lattice. The curve has a linear part of slope $D \approx 2.35$ over approximately two decades.

to the surface and satisfying the self-avoiding constraints. We present evidence that the fractal dimension is exactly 3 in this model, just as in the usual Eden model in three dimensions (Richardson 1973, Dhar 1985, Leyvraz 1985), so that the constraint that the surfaces be locally two-dimensional is irrelevant for the ESAS.

One thousand growing Eden surfaces of size 10^4 have been simulated on a $101 \times 101 \times 101$ cubic lattice. The surfaces obtained for ESAS are much more compact than those for DLSAS, as can be seen in figure 2. In fact, we were able to grow a series of 10 surfaces containing 5×10^4 plaquettes without reaching the boundaries of a $91 \times 91 \times 91$ lattice. In figure 3 a plot of ln (R_g) against ln (N) is shown. A linear extrapolation

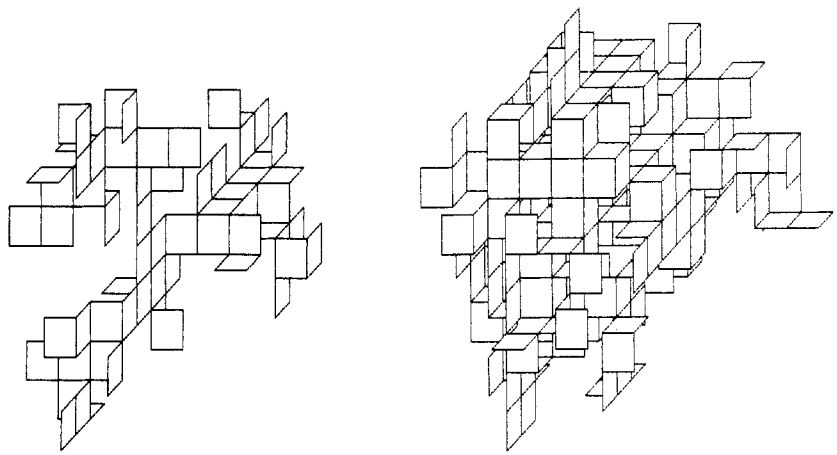

Figure 2. Two typical surfaces grown until the boundaries of a $15 \times 15 \times 15$ cubic lattice are reached. The diffusion-limited surface (*a*) contains 71 plaquettes and is much more ramified than the Eden surface (*b*) which contains 224 plaquettes.

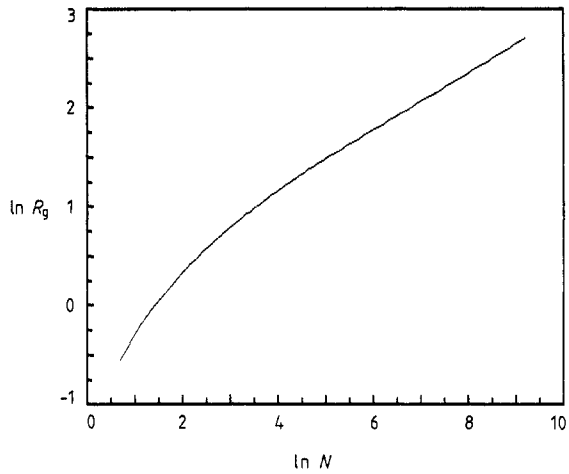

Figure 3. A plot of ln R_g against ln N for the Eden self-avoiding surfaces. A linear fit of the rightmost part of the curve gives a slope $D \approx 3.3$, showing that the asymptotic regime has not yet been reached.

of the rightmost part of the curve would give a fractal dimension of about 3.3, which shows that, even for such large N values, we are still in a transient regime. However, the evolution of the fractal dimension D with N can be obtained using an effective exponent

$$D_i(N) = \ln\{(N+i)/(N-i)\}/\ln\{R_g(N+i)/R_g(N-i)\}$$

where $R_g(N)$ is the mean radius of gyration for the surfaces of size N and i a fixed positive integer. In figure 4, which shows $D_5(N)$ as a function of ln (N), we can see that convergence of the fractal dimension toward $D = 3$ for higher values of N is very probable. Completely analogous behaviour is observed for the usual Eden model (Peters *et al* 1979).

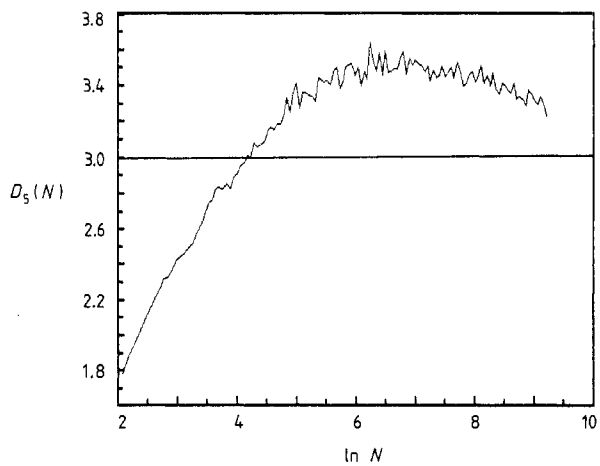

Figure 4. The variation of the effective fractal dimension $D_5(N)$ as a function of ln N for the ESAS. Gradual convergence toward $D = 3$ is apparent.

Unlike in the DLSAS, termination of the growth process by trapping can occur for the ESAS. For the kinetic self-avoiding walk (Majid *et al* 1984, Lyklema and Kremer 1984)—an Eden growth model for self-avoiding walks (SAW)—a crossover toward the equilibrium SAW which is due to non-local trapping has been predicted (Peliti 1984, Pietronero 1985) and was subsequently observed in numerical simulations (Lyklema and Kremer 1986). For the ESAS, however, there is no obvious reason why trapping would produce a crossover to the equilibrium self-avoiding surface, with $D=2$. Moreover, our numerical results are highly incompatible with a value of two for the fractal dimension.

We have also considered the growth of the ESAS perimeter. A surface containing N plaquettes was found to have N_p empty perimeter faces with $N_p \sim N^{0.8}$ and the perimeter radius of gyration scaled as $R_p \sim N_p^{1/3}$, as for the bulk. These exponents are still likely to vary, since asymptotic N values have not yet been reached.

In conclusion, we have performed Monte Carlo simultations of two models of growing self-avoiding surfaces. The growing surfaces were constrained to be locally planar. This local constraint has been shown to be relevant when the growth is diffusion limited (DLSAS), and we find a fractal dimension $D=2.35\pm0.05$ in this case. On the other hand, when the growth is of the Eden type (ESAS) the constraint appears to be irrelevant and we obtain compact surfaces.

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