

FORMATION OF DNA NETWORKS — COMPUTER SIMULATIONS*

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We report results of the computer simulation of the kinetic gelation process of the formation of a two-dimensional network. The simulation is performed on a basis of a two-dimensional triangular lattice. Our aim is to analyze the distribution $N_g(s)$ of the pore size s in the network, as dependent on the concentration of the linear polymer molecules in the system. Here we demonstrate, that for some critical concentration of the molecules the obtained distribution is close to $N_g(s) \propto s^{-\tau}$ and it does not depend on the probability of merging. The obtained value of the exponent τ agrees with the result for clusters in the theory of percolation on the two-dimensional lattice.

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1. Introduction

Continuous search for potential applications of DNA is motivated by special features of the DNA molecules. They are known to carry the genetic information for life, but relations of their structure and particular biological functions is not known. Their ability to associate with other DNA molecules by means of specific base pairing mechanism [1] is much simpler to describe, but research on possible consequences of this ability remain at an introductory level. More than 50 years after the discovery of the double-helical structure of DNA, possibilities of using DNA as new nanomaterials are surprisingly rich [2, 3].

In particular, it is possible to construct spatial structures of DNA. These structures can be spatially ordered, as two-dimensional arrays [4, 5] or three-dimensional crystals [6, 7], or disordered. Ordered DNA crystals can be

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used as molecular sieves [7]. Here we are motivated by a question if disordered structures can also play this role. Then, the pore size distribution of such a structure is of interest. The process simulated is equivalent to the irreversible kinetic gelation [8–10]. Up to our knowledge, the pore size distribution has not been investigated there.

In a recent paper [11] we calculated the distribution of the pore size of a two-dimensional random network, as dependent on size and density of the DNA molecules which formed the network. The system was a set of molecules which initially move in a triangular lattice, as in a lattice-gas model [12] (although we prefer to imagine that the medium is rather a liquid than a gas). Basically, two kinds of molecules should be used: linear and branched. However, in our simulation the only role of the branched molecules is just to enable the linear molecules to merge. Then, in fact the branched molecules are absent in the simulation. Doing the calculations, we assumed that at each time step the merging occurred with probability one [11]. This assumption was motivated by saving the computational time. However, it is not realistic, as in any many-body system the probabilistic description is known to be more appropriate. In principle, this assumption can also modify the character of the processes, as some information on the initial structure can be preserved artificially if the process of merging is too intense. Then we released the above assumption and carried out the calculations. The aim of this paper is to report the results.

2. Calculations

The simulation is performed on a basis of two-dimensional triangular lattice with a lattice constant a . The size of the lattice was 512×512 . The simulations were made for different lengths $L(a - 9a)$ and different number $N(1 \times 10^4 - 9 \times 10^4)$ of the linear molecules. Initial positions of the linear molecules (with given values of N and L) were chosen randomly with three possible orientations given by the structure of the lattice. During the simulations the linear molecules can move along their axis, with equal probabilities for both possible directions. When two linear molecules met at a lattice node, they are merged with different probabilities ρ for different computer experiments. This is an equivalent of different concentrations ρ of the branched molecules. The maximal number of the linear molecules at any node of the lattice was arbitrarily established to three (which is simultaneously the number of arms of the branched molecules). In this way, we introduce the limitation of excluded volumes to the model. At the beginning there is a lot of free linear molecules in the system. At each step of the simulation the number of the free molecules decreases, as most of them get attached. However, the probability ρ remains fixed within a given simulation. Its value is taken from 0.1 to 1.0. The procedure enables to set

a number of the simulation steps after which the system does not change. Then, the amount of the linear molecules which remain free does not exceed 1 per 100. We checked that this condition is met when the number of steps for all simulations was set to 100. At each step, all movable molecules made an attempt to move. The results are averaged over 10 independent simulations.

3. Results and discussion

Here we analyze the distribution of the pore sizes $N_g(s)$ in the network, as dependent on the number N of molecules per cell in the system. By the term “pore size” we mean the number of free neighbouring nodes of the lattice. As we reported in our previous work [11], the character of the pore size distribution varies depending on the values of the N and L . When the system is dilute (for short molecules and low concentrations of the linear molecules) big isolated pores are present. For intermediate values of N and L the $N_g(s)$ curve in double-logarithmic scale becomes approximately a straight line (a critical behaviour). Finally, for large values of N and L (a dense system) the order of the magnitude of largest pore sizes s decreases from 10^2 to 10 and the relation is no more a power law. Analysis of the distribution of the pore size of the networks obtained for different values of the length and the number of linear molecules in the system allowed [11] to construct a phase diagram (N, L) (see Fig. 1). On this diagram we can schematically mark a line near which the distribution of the pore size is a power law $N_g(s) \propto s^{-\tau}$ (critical). Above this line the system is dense and below the line it is dilute.

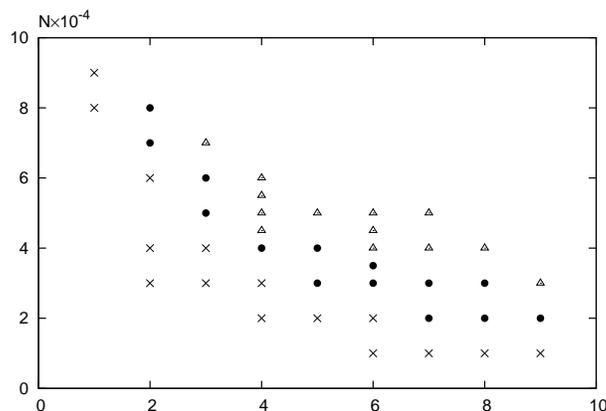


Fig. 1. The phase diagram of the state of the network; where: \times denotes dilute system, \bullet — critical behaviour and Δ — dense system. The fuzzy character of the critical line (two or more points marking the critical character for the same L) can be a finite-size effect. The diagram is an improved version of Fig. 5 of Ref. [11].

In Fig. 2, we show the results of the calculations of $N_g(s)$ for $\rho = 0.1, 0.3, 0.6, 0.9$ and 1.0 . As we see, the obtained points form the same plot, except some spread at largest values of s . This means, that the pore size distribution does not depend on the probability ρ of the merging. As this probability controls the velocity of the formation of the network, we can conclude that this velocity is not relevant. This means that the obtained structure does not carry an information on the initial stage; we can speak about some unique state, analogous to the equilibrium state in the statistical mechanics.

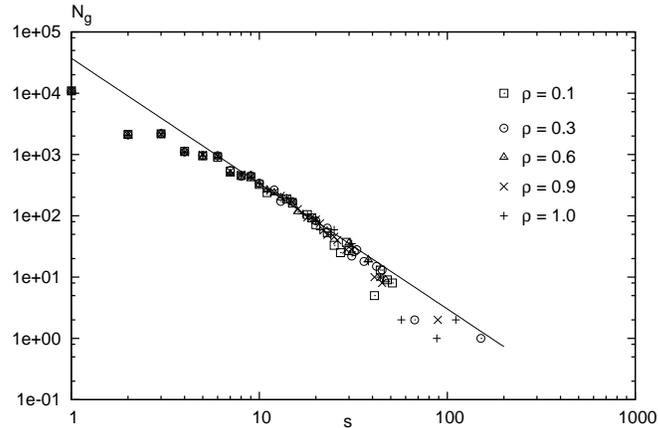


Fig. 2. The pore size distribution $N_g(s)$ for various concentrations ρ of the branched molecules. The number of the linear molecules $N = 3 \times 10^4$, and their length is $L = 7a$. The solid line is the fit to the central part of the plot; its slope gives $\tau = 2.04 \pm 0.05$.

Additionally, the superposition of the plots obtained for four values of ρ improved the statistics with respect to the results reported in Ref. [11]. Central part of the plot fitted by the function $s^{-\tau}$ gave the value $\tau = 2.04 \pm 0.05$. The error of this fitting should be multiplied by a factor 2 or 3 because of the ambiguity of the selection of the central part of the plot. Nevertheless, the obtained value nicely agrees with theory of percolation on the square lattice, which gives $\tau = 187/91$ [13, 14]. We note that this theory deals with the distribution of clusters, and not of the free spaces. This result suggests the symmetry cluster-free space, which holds despite the fact, that the one state of an empty cell cannot be projected into more states of an occupied cell.

Concluding, the pore size distribution in the DNA network formed in the kinetic gelation process varies from the regime of large pores to the one of small pores through an intermediate (critical) state, where the distribution is close to the scale-free one. The pore size distribution in the intermediate

state is close to the result predicted by the percolation theory. We note, that this result should be confirmed by simulations for larger lattices. We note also that our simulation is not limited to DNA, but it can be equally applied to other kinds of linear molecules.

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