# Static and dynamic properties of the backbone network for the irreversible kinetic gelation model

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We study by Monte Carlo simulations the fractal nature of the backbone network for the irreversible kinetic gelation model in both two and three dimensions. The fractal dimension of the backbone network generated at the gel point is measured by various methods, and results are found to be consistent with that of the standard percolation backbone. Our observation is different from the previous work in three dimensions, where a distinctly larger value was observed. We also measure the spectral dimension  $d_s^B$  and the fractal dimension  $d_w^B$  of random walks on a backbone, defined by, respectively, the probability of random walks returning to the starting point and the rms displacements after *t* time steps. Results are also found to be consistent with the corresponding percolation values. We therefore conclude that the backbone network of the kinetic gelation model exhibits the same static and dynamic properties as those of the standard percolation backbone.

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# I. INTRODUCTION

Kinetic gelation is the irreversible growth model designed to investigate formation of an infinite macromolecule. The initial study of the sol-gel transition was carried out by Flory and Stockmayer [1,2] using a simple model, later known as percolation on a Bethe lattice. A more realistic model of an additive copolymerization by radicals has been developed by Manneville and de Seze [3]. In such a model, all lattice sites are assumed to be initially in a sol phase, which consists of small monomers of multiple functionalities. The gelation is initiated by radicals which saturate, opening up a double bond of a monomer and leaving one bond of the monomer unsaturated. The unsaturated bond acts as a new radical which, in turn, opens up another double bond of the neighboring monomer. As this process continues, an infinite macromolecule occurs suddenly at a certain fraction of the polymerized sites, known as the gel-point  $p_c$ . A typical example of such a gelation phenomenon can be viewed from the formation of the macromolecule by acrylamide initiated by ammoniumsulfate, as described in Ref. [4].

The universality of the kinetic gelation model has been intensively studied, particularly in three dimensions (3D), by Herrmann *et al.* [4,5]. They found that the critical exponents  $\gamma$  and  $\nu$ , which characterize, respectively, the percolation susceptibility and the correlation length, are roughly the same as the corresponding lattice percolation values. However, the amplitude ratio *R* of percolation susceptibilities below and above  $p_c$ , which is supposed to be universal [6], has been found to be considerably smaller than that of the percolation value. Based on this observation, they claimed that the kinetic gelation model belongs to a different universality class from that of the lattice percolation. In 2D, on the other hand, both the exponents  $\gamma$  and  $\nu$  and the amplitude ratio *R* were found to be considerably different from the percolation counterparts [7], again suggesting different universality classes. The fractal dimension of an infinite network was also determined considerably larger than that of the percolation network [8], though it was later found by a more elaborate technique to be similar to the percolation value [9].

Considering these works, it appeared that, while the critical exponents of the gelation model were similar to those of the percolation counterparts, the amplitude ratio R was still different. Similar results were also reported for other percolation models such as the off-lattice, randomly bonded percolation and the continuum percolation models [10–12].

Recently, Lee and his collaborators [13–16] intensively studied the amplitude ratio of percolation susceptibilities for various off-lattice percolation models and the kinetic gelation model. They found that the nonuniversal behaviors of the amplitude ratio reported earlier for various models had been caused artificially by different sampling techniques for the percolation susceptibilities in the Monte Carlo procedure. After minimizing the errors, the amplitude ratio of percolation susceptibilities for various models was found to be consistent with the known lattice percolation value, implying a strong universality between lattice percolation and other aforementioned models.

However, it is still unclear whether or not the static and dynamic properties of the *backbone* network for the kinetic gelation model are also similar to those of the percolation backbone. The fractal dimension of such a backbone was in fact reported to be distinctly larger than that of the percolation backbone [17]. Since the fractal dimension  $d_F$  of an infinite percolation network at criticality is related to the critical exponents  $\nu$  and  $\beta$ , characterizing, respectively, the correlation length and the order parameter, via

$$d_F = d - \beta / \nu, \tag{1}$$

*d* being the spatial dimensionality, obtaining different fractal dimensions implies that two models belong to different universality classes. A similar argument is valid for the backbone network as well, with the exponents characterizing those quantities of the backbone. The backbone is an infinite

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network obtained by eliminating all dangling loops and dead ends which do not carry current when the electric potential is applied between two opposite edges or faces. The backbone at  $p_c$  is known to exhibit a self-similar structure with its fractal dimension different from that of the infinite network and plays a crucial role in determining the dynamical properties such as the electrical conductivity, permeability, and elastic properties. It is, thus, interesting to study the fractal nature of the backbone network at criticality for the kinetic gelation model.

In this work, we study the fractal nature of the backbone network of an infinite cluster generated at the gel point for the kinetic gelation model. We measure the fractal dimension  $d_F^B$  from the mass distributions of monomers and from the fraction of monomers on the backbone. We also estimate the two indices regarding the random walks on a backbone, the spectral dimension  $d_s^B$ , and the fractal dimension  $d_w^B$  characterizing, respectively, the probability of returning to the starting point and the rms displacements. With these estimates, the fractal dimension of the backbone is also calculated using the Alexander-Orbach scaling relation [18].

### **II. MONTE CARLO PROCEDURE**

The Monte Carlo method of obtaining realizations for the kinetic gelation model is basically the same as that described in Ref. [16]. At the beginning of each simulation step, all lattice sites on a system of a side L are assumed to be in the sol phase, no solvent molecule being assumed to exist, with the fractions of the tetrafunctional units  $c_t$  and the bifunctional units  $c_b$ . The initiators of concentration  $c_l$  are randomly distributed in a given system, assuming that each initiator acts as an active center for polymerization. Then, one of those active centers and its neighboring bond are selected randomly. If the new site connected by that bond is not yet saturated, i.e., has fewer than 2d incident bonds, the bond is completed and the active center is moved to a new site. If the bond cannot be completed by the neighboring sites being saturated with 2d bonds, a new attempt is made with different active center.

Once the realization is obtained at the gel point, we search for an "incipient" infinite cluster which spans the cell along *all* coordinate directions, using the cluster labeling algorithm [19]. If such a cluster does not exist, we discard the current realization and attempt a new realization. If such an infinite cluster is found, we set all sites other than the sites on an infinite cluster to be zero. The backbone is then extracted using the Roux-Hansen algorithm [20] for two dimensions (2D) and the so-called "burning" algorithm [21] for 3D. The Roux-Hansen algorithm is much simpler and more efficient than the burning algorithm, but it can only be applied for a 2D model because of the spatial characteristics. A sample realization generated on a  $50 \times 50$  square lattice is shown in Fig. 1.

Once the desired backbone is extracted, we calculate the monomer distributions on the backbone against the distance from the randomly selected points and also the fraction of monomers on it, i.e., the gel fraction. We also generate random walks from the randomly selected starting points on the backbone and calculate the number of events in which random walks return to the starting points and the rms displace-



FIG. 1. Computer-generated sample realization of (a) an infinite network and (b) a backbone network extracted from (a) for the kinetic gelation model on a  $50 \times 50$  square lattice.

ments after t time steps. These quantities enable us to estimate the spectral dimension  $d_s^B$  and the fractal dimension  $d_w^B$  of random walks on a backbone.

## **III. RESULTS AND DISCUSSION**

We carry out simulations for the kinetic gelation on  $L^d$  lattice sites for various values of L and for selected values of  $c_I$  and  $c_t$  for which the gel points were reported. The results are averaged over at least 100 realizations.

#### A. Fractal dimension from the mass distribution

We calculate the number of monomers on a backbone inside the circle (sphere for 3D) of radius r, centered at the randomly selected point. Assuming that each monomer has a mass of unity, the mass of monomers on a backbone inside the circle (sphere) of radius r is expected to increase as

$$M(r) \sim r^{d_F^B} \tag{2}$$

for  $r \ge a$ , where *a* is the lattice constant. Whenever each center of the circle (sphere) is selected, we reconstruct the



FIG. 2. Plots of M(r) against r on a double logarithmic scale for the backbone network of the kinetic gelation model for  $c_I = 0.05$ (circles) and 0.2 (squares) in 2D, obtained using the two different boundary conditions. The upper set is the data for periodic boundaries and the lower set for free boundaries. Note that the data for periodic boundaries were multiplied by a factor of 10 to avoid overcrowding of the symbols.

backbone realization by translating the center of the circle (sphere) to the center of the system by periodic boundary conditions. We then redetermine the connectivity and count the number of occupied sites inside the circle (sphere) by varying the radius r from r=a up to r=La/2. In this final stage, we employ the two different boundary conditions, the free and the periodic boundaries. In general, the periodic boundaries yield an estimate of the fractal dimension slightly larger than what the free boundaries would yield.

Plotted in Fig. 2 are the data for the 2D kinetic gelation model generated on a 1001×1001 square lattice for  $c_I$ =0.05 (circles) and 0.2 (squares), assuming that all sites are occupied with monomers of the tetrafunctional units, i.e.,  $c_{t}$ =1. The upper sets are those obtained using the periodic boundaries and the lower sets using the free boundaries. The upper data are shifted by an amount 1.0 to avoid overcrowding of the data. As shown in the figure, the data for two different values of  $c_1$  are not appreciably different, indicating that the fractal dimension of the backbone network is independent of the concentration of initiators. The estimates of the fractal dimension from the plot are  $d_{F,p}^B = 1.65 \pm 0.01$  for periodic boundaries and  $d_{F,f}^B = 1.60 \pm 0.01$  for free boundaries. It is generally known that the periodic boundaries yield a fractal dimension that is slightly overestimated, while the free boundaries vield an underestimation of the fractal dimension. Thus, the true value of the fractal dimension is expected to lie between the two estimates. It should be noted that the known fractal dimension of the backbone network for ordinary lattice percolation,  $d_F^B = 1.647 \pm 0.004$  [22,23], lies between the two values.

Plotted in Fig. 3 on a double logarithmic scale are the data in 3D for L=181 and  $c_I=0.0003$  with  $c_I=1.0$ . Again the upper sets are from the periodic boundary condition and are



FIG. 3. As in Fig. 2 for the 3D kinetic gelation model for  $c_I = 0.0003$  and  $c_t = 1.0$ , using the periodic boundaries (squares) and the free boundaries (circles). The data for periodic boundaries are multiplied by a factor of 10.

shifted by an amount 1.0, and the lower sets are from the free boundary condition. The linear regression fits yield estimates of the fractal dimension  $d_{F,p}^B = 1.859 \pm 0.011$  for periodic boundaries and  $d_{F,f}^B = 1.857 \pm 0.010$  for free boundaries. These values are again close to the known lattice percolation value in 3D  $d_F^B = 1.855 \pm 0.015$  [24].

### B. Fractal dimension from the gel fraction

Since the estimates of the fractal dimension from the mass distribution of the monomers on a backbone depend on the boundary conditions employed, it is still less clear whether or not the fractal dimension of the backbone network of the kinetic gelation model is the same as that of the ordinary lattice percolation value. In order to derive a more conclusive answer, we also measure the fraction of the monomers on the backbone network.

The gel fraction G(p,L) of the backbone is the fraction of the monomers on the backbone in a given system of side Land is related to the number of monomers M(p,L) as  $G(p,L)=M(p,L)/L^d$ . Since the gel fraction for any finitesize system is known to satisfy the scaling relation [25]

$$G(p,L) \sim L^{-\beta_B/\nu} f(|p-p_c|L^{1/\nu}), \qquad (3)$$

near the gel point, it can be written at  $p = p_c$  as

$$G(p_c, L) \propto L^{-\beta_B/\nu}.$$
 (4)

The fractal dimension  $d_F^B$  can thus be obtained from  $M(p_c,L) = L^d G(p_c,L) \propto L^{d_F^B}$  as

$$d_F^B = d - \beta_B / \nu. \tag{5}$$

Therefore, the fractal dimension of the backbone network is obtained by estimating  $\beta_B/\nu$  from the gel fraction for various sized systems.



FIG. 4. Plots of the gel fraction on a backbone against the linear size of the system for the kinetic gelation model for  $c_1 = 0.05$  (upper data) and  $c_1 = 0.2$  (lower data) in 2D. The closed symbols are the data obtained from the periodic boundaries, the open symbols from the free boundaries, and the solid lines are the regression fits. The upper sets of data are shifted by an amount of 0.3 to improve the readability.

Shown in Fig. 4 are the gel fractions, plotted on a double logarithmic scale against the size of system L ranging from 30 to 1000, for  $c_1 = 0.2$  (circles) and  $c_1 = 0.05$  (squares) in 2D. The closed symbols are the data from the periodic boundaries and the open symbols from the free boundaries. (Note that the upper sets are shifted by 0.3 to improve readability.) The solid lines are the regression fits, which yield the estimates  $\beta_B/\nu = 0.354 \pm 0.002$  for  $c_I = 0.2$  and  $\beta_B/\nu$  $=0.349\pm0.007$  for  $c_1=0.05$ . These values are the averages of the estimates from the two different boundary conditions. From these values, the fractal dimension of the backbone network is estimated, using Eq. (5), as  $d_F^B = 1.646 \pm 0.004$ and  $d_F^B = 1.651 \pm 0.014$  for  $c_I = 0.2$  and 0.05, respectively. These values are consistent, within statistical errors, with the value obtained from the mass distribution using the periodic boundary condition, and they are also consistent with the fractal dimension of the backbone of the ordinary percolation.

Shown in Fig. 5 are the 3D data of the gel fraction for  $c_I = 0.003$  (closed circles), in comparison with the corresponding data for the backbone of the ordinary lattice percolation at percolation threshold  $p_c = 0.3117$  (open circles), plotted against the size of system *L* ranging from 10 to 180. The upper sets of data are obtained using the periodic boundaries and are shifted by an amount 1.0, and the lower sets are obtained using the free boundaries. We also carried out simulations for  $c_I = 0.003$  and found that the plots were basically similar to those for  $c_I = 0.03$  (not shown). The mean estimates of the regression fits from two boundary conditions for the kinetic gelation model yield the slope  $\beta_B/\nu = 1.143 \pm 0.005$  for  $c_I = 0.003$  and  $1.146 \pm 0.002$  for  $c_I = 0.03$ , which, respectively, yield the fractal dimension  $d_B^F = 1.857 \pm 0.010$  and  $1.854 \pm 0.004$ . On the other hand, the corresponding es-



FIG. 5. Plots of the gel fraction on a backbone against the linear size *L* of the system for the kinetic gelation model for  $c_I = 0.003$  in 3D (closed symbols), in comparison with the corresponding data for the percolation backbone (open symbols). The upper sets are the data obtained using the periodic boundaries, the lower sets from the free boundaries, and the solid lines are the regression fits. Note that the upper sets of data are multiplied by 10.

timate for lattice percolation is  $\beta_B/\nu = 1.142 \pm 0.004$ , which, accordingly, yields  $d_F^B = 1.858 \pm 0.008$ , which is consistent with the known value [24] and is also consistent with the estimates for the gelation model.

We have so far measured the fractal dimension of the backbone network for the kinetic gelation model both in 2D and 3D. The fractal dimensions were found to be independent of the initiator concentration and were close to the lattice percolation values for both dimensions. This observation assures us that the static properties of the backbone network for the kinetic gelation model are similar to those of the ordinary lattice percolation.

# C. Random walks on a backbone network

Although we obtained a fractal dimension of the backbone network for the kinetic gelation model similar to that of the percolation backbone, we are still uncertain of the dynamic properties of the backbone. The dynamic properties may depend on the substrate structure in a more complex manner. As an example, an infinite network of continuum percolation exhibits all the static properties similar to those of the ordinary lattice percolation; however, the conductivity exponent in 3D was found to be different from the corresponding lattice percolation value [26]. It is, therefore, interesting to study the dynamic properties of the backbone network to clarify the universality of the kinetic gelation model.

In order to investigate the dynamic properties of the backbone, we generate random walks from the randomly selected starting points on a backbone and calculate the probability P(t) of returning to the starting point and the rms displacement  $\langle R(t)^2 \rangle^{1/2}$  after t time steps. The probability P(t) behaves asymptotically as



FIG. 6. Plots of P(t) against t for random walks on a backbone of the kinetic gelation model. The lower data are the 2D results for  $c_I = 0.05$  and the upper data the 3D results for  $c_I = 0.003$ . The solid lines are the regression fits, with the slope equal to  $-d_s^B/2$ .

$$P(t) \sim t^{-d_s^B/2},\tag{6}$$

 $d_s^B$  being the spectral dimension of the backbone, which is also related to the density of states for the lattice vibration of frequency  $\omega$  via  $\rho(\omega) \sim \omega^{d_s^B - 1}$ , while the rms displacement  $\langle R(t)^2 \rangle^{1/2}$  is known to exhibit the asymptotic behavior as

$$\langle R(t)^2 \rangle^{1/2} \sim t^{1/d_w^B},\tag{7}$$

 $d_w^B$  being the fractal dimension of random walks on a backbone network.

In order to estimate the spectral and fractal dimensions of random walks, we calculate the probability P(t) and the mean-square displacement  $\langle R(t)^2 \rangle$  up to 50 000 time steps. The raw data of P(t) obtained from the simulation exhibit strong even-odd oscillations, which are attributed to the characteristic of the underlying lattice structure. In order to get rid of such oscillations, we calculate the average of the data in every interval of  $\Delta(\ln t)=0.05$  and plot the result on the geometrical average time in each interval. Shown in Fig. 6 are such data for random walks on a backbone in 2D for  $c_I = 0.05$  and  $c_I = 1$  (lower data) and in 3D for  $c_I = 0.003$  and  $c_I = 0.4$  (upper data). In both plots, data for  $t \ge 100$  yield a good power-law behavior, indicating that P(t) indeed behaves as in Eq. (6).

In 2D, the linear regression fit between 100 and 50 000 time steps yielded the slope  $d_s^B/2=0.622\pm0.005$ . We also calculated the same quantities for other values of  $c_I$ ,  $c_I = 0.01$ , 0.02, 0.1, and 0.2, all with  $c_t=1$ . All plots are basically similar to that in Fig. 6 with the regression slope of  $d_s^B/2=0.624\pm0.003$ , which is consistent with the estimate for  $c_I=0.05$ . From these estimates, we obtain the spectral dimension  $d_s^B=1.246\pm0.010$ . This value is larger by about 2% than the corresponding value on a backbone network of the ordinary lattice percolation,  $d_s^B=1.22\pm0.02$ , which is



FIG. 7. Plot of  $[d_{w,\text{eff}}^B(t)]^{-1}$  for random walks on a backbone of the kinetic gelation model for selected values of  $c_I$  in 2D. The inset is the plot of the same data for late time.

estimated from the known values of  $d_w^B$  and  $d_F^B$  [27] by the Alexander-Orbach scaling relation  $d_s^B = 2d_F^B/d_w^B$  [18]. However, since the difference is small and the errors overlap one onto another, we still believe that they are consistent with each other, implying that the spectral dimension of the backbone of the kinetic gelation model is similar to the percolation backbone. (To the best of our knowledge, no reliable data for  $d_s^B$  of random walks on a percolation backbone are available as yet.)

In 3D, calculations for  $c_I = 0.03$  and  $c_i = 1.0$  are also carried out, in addition to that presented in Fig. 6. The linear regression fit between 100 steps and 25 000 steps yielded the slope  $d_s^B/2=0.589\pm0.002$  for  $c_I=0.003$  and  $c_t=0.4$  and  $d_s^B/2=0.592\pm0.001$  for  $c_I=0.03$  and  $c_t=1.0$ . From these estimates, the spectral dimension is estimated to be  $d_s^B = 1.181\pm0.010$ . This is again consistent with the value of  $d_s^B = 1.18\pm0.01$  for a backbone network of the standard percolation model [24].

In order to estimate the fractal dimension of random walks  $d_w^B$  on a backbone, one should plot, as for P(t),  $\langle R(t)^2 \rangle$  against t on a double logarithmic scale and estimate the asymptotic slope in the  $t \rightarrow \infty$  limit. However, if the rms displacement exhibits nontrivial correction terms, as in Eq. (7), estimating  $d_w^B$  will not be as simple as for  $d_s^B$ . In order to measure  $d_w^B$  accurately, we define the effective index  $[d_{w,\text{eff}}^B(t)]^{-1}$ , similar to  $\nu_{\text{eff}}(t)$  in Ref. [28], which results in, using Eq. (7),

$$[d_{w,\text{eff}}^{B}(t)]^{-1} = 1/d_{w}^{B} + at^{-\Delta} + bt^{-1} + \cdots, \qquad (8)$$

where  $\Delta$  is the possible nonanalytic correction-to-scaling exponent. In order to extract the fractal dimension of random walks, it is natural to plot  $[d_{w,eff}^{B}(t)]^{-1}$  against  $t^{-1}$  and extrapolate the value in the  $t^{-1} \rightarrow 0$  limit.

Shown in Fig. 7 is the  $[d_{w,\text{eff}}^B(t)]^{-1}$  plotted against  $t^{-1}$ , for random walks on a backbone network of the 2D kinetic gelation model, the inset being the plot of large *t* regions. Plots for  $c_I = 0.05$ , 0.1, and 0.2 appear to converge onto the



FIG. 8. As in Fig. 7 for the 3D kinetic gelation model for  $c_I = 0.03$  ( $c_t = 1.0$ ),  $c_I = 0.003$  ( $c_t = 0.4$ ), and  $c_I = 0.0003$  ( $c_t = 1.0$ ).

same value in the  $t^{-1} \rightarrow 0$  limit. On the other hand, data for  $c_I = 0.02$  and 0.01 appear to show slow convergence behavior. This might be because the substrate fractal is less compact than those of the larger values of  $c_I$ , and random walks encounter more friction than for the cases of larger  $c_I$ . Indeed, the gel-points for these two cases are lower than the other cases. However, the upturns near the end of the chain clearly indicate that they converge asymptotically onto the same value on the ordinate. Simple extrapolation of the plot yields  $1/d_w^B = 0.381 \pm 0.010$ , i.e.,  $d_w^B = 2.64 \pm 0.01$ , which is not inconsistent with the corresponding lattice percolation value  $d_w^B = 2.69 \pm 0.04$  [27].

The fractal dimension of the substrate backbone can also be obtained from the estimates of  $d_s^B$  and  $d_w^B$  as

$$d_F^B = d_s^B d_w^B / 2 = 1.645 \pm 0.010$$

which is in excellent agreement with the earlier estimate.

In 3D, the results are basically similar to those in 2D. Data for smaller  $c_I$  such as those for  $c_I=0.0003$  ( $c_t=1.0$ ) and 0.003 ( $c_t=0.4$ ) are smaller than those for larger  $c_I$ , as shown in Fig. 8. However, beyond 5000 time steps, data for both cases exhibit a sharp upturn. Considering the data for three cases, it appears that the value of  $[d_{w,eff}^B(t)]^{-1}$  converges onto a value of  $1/d_w^B \approx 0.32$ , which is also consistent with that of the random walks on a percolation backbone,  $d_w^B = 3.13 \pm 0.03$  [24]. It is thus clear that the fractal dimension of random walks on a backbone network in 3D is also similar to the corresponding percolation value.

Another possible way to confirm this is to estimate  $d_w^B$  from the Alexander-Orbach scaling relation. With the previous estimates of  $d_s^B$  and  $d_F^B$  in 3D, one can calculate  $d_w^B$  as

$$d_w^B = 2d_F^B/d_s^B \simeq 3.14$$

which is consistent with our estimate.

We also employed the Markov chain analysis of random walks [29] on a backbone network. The transition probability matrix **W** and its dominant eigenvalues are calculated. The

spectrum of the eigenvalues is related to the spectral and fractal dimensions of random walks via the Laplace transform. One of the advantages of such an analysis is that the detailed zigzag motion of random walks is not necessary; however, the estimate appears not to be as accurate as that of the direct Monte Carlo analysis. As a cross check, we calculated the eigenvalues of the transition probability matrix and estimated the spectral and fractal dimensions of random walks on a backbone for  $c_1 = 0.2$ . Results were found to vary depending on the size of the system; the raw estimates are  $d_s^B = 1.230 \ (L = 250), \ 1.234 \ (L = 200), \ 1.237 \ (L = 150), \ and$ 1.240 (L=100), and  $d_w^B=2.693$  (L=250), 2.705 (L= 200), 2.708 (L=150), and 2.712 (L=100). A similar size dependence was recently found by Lee and Nakanish for random walks on an infinite network of 4D percolations in a hypercubic lattice [30]. Considering the size dependence, we obtained  $d_s^B = 1.22 \pm 0.01$  and  $d_w^B = 2.69 \pm 0.01$ , both of which are also in agreement with those of random walks on a percolation backbone.

#### **IV. SUMMARY AND CONCLUSIONS**

We studied by Monte Carlo simulations the fractal nature of the backbone network for the irreversible kinetic gelation model. The fractal dimension of the backbone network generated at the gel point was measured by various methods, and the results were found to be consistent with that of the backbone of the standard percolation model. Our observation is different from the previous work in 3D, where a distinctly larger value was observed. We also measured the spectral dimension  $d_s^B$  and the fractal dimension  $d_w^B$  of random walks on a backbone defined, respectively, by the probability of random walks returning to the starting point and by the rms displacements after t time steps, and we obtained  $d_s^B$  $= 1.246 \pm 0.010$  and  $d_w^B = 2.64 \pm 0.01$  in 2D and  $d_s^B = 1.181$  $\pm 0.010$  and  $d_w^B = 3.13 \pm 0.01$  in 3D. These values are consistent, within the statistical errors listed, with the corresponding percolation values. From these observations, we conclude that both the static and dynamic properties of the backbone network for the kinetic gelation model are similar to those of the percolation backbone and the two models belong to the same universality class.

It is interesting that the two models generated by different procedures exhibit the same critical behavior. While the percolation is the *static* equilibrium model, the gelation is the *irreversible growth* model where bonds are formed as a result of a kinetic growth process. Our results suggest that the "static" percolation model may be adequate to describe the sol-gel transition and related phenomena of the irreversible growth model.

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- [1] P.J. Flory, J. Am. Chem. Soc. 63, 3083 (1941).
- [2] W.H. Stockmayer, J. Chem. Phys. 11, 45 (1943).
- [3] P. Manneville and L. de Seze, in *Numerical Methods in the Study of Critical Phenomena*, edited by I. Della Dora, J. Demongeot, and B. Lacolle (Springer, Berlin, 1981).
- [4] H.J. Herrmann, D. Stauffer, and D.P. Landau, J. Phys. A 16, 1221 (1983).
- [5] H.J. Herrmann, D.P. Landau, and D. Stauffer, Phys. Rev. Lett. 49, 412 (1982).
- [6] A. Aharony, Phys. Rev. B 22, 400 (1980).
- [7] A.F. Rushton, F. Family, and H.J. Herrmann, J. Polym. Sci., Polym. Symp. 73, 1 (1985); also see A. F. Rushton, M.S. thesis, Emory University (1984).
- [8] F. Family, Phys. Rev. Lett. 51, 2112 (1983).
- [9] D.C. Hong, H.E. Stanley, and N. Jan, Phys. Rev. Lett. 53, 509 (1984).
- [10] D.Y. Kim, H.J. Herrmann, and D.P. Landau, Phys. Rev. B 35, 3661 (1987).
- [11] I. Balberg, Phys. Rev. B 37, 2391 (1988).
- [12] S.B. Lee and S. Torquato, Phys. Rev. A 41, 5338 (1990).
- [13] S.B. Lee, Phys. Rev. B 42, 4877 (1990).
- [14] S.B. Lee and J.H. Ahn, J. Korean Phys. Soc. 26, S438 (1993).
- [15] S.B. Lee, Phys. Rev. E 53, 3319 (1996).
- [16] S.B. Lee and H. Jeon, Phys. Rev. E 56, 3274 (1997).

- [17] A. Chhabra, H. J. Herrmann, and D. P. Landau, in *Fractals in Physics*, edited by L. Pietronero and E. Tosatti (Elsevier Science Publishers, Amsterdam, 1986).
- [18] S. Alexander and R. Orbach, J. Phys. (France) Lett. 53, 625 (1982).
- [19] J. Hoshen and R. Kopelman, Phys. Rev. B 14, 3438 (1976).
- [20] S. Roux and A. Hansen, J. Phys. A 20, L1281 (1987).
- [21] H.J. Herrmann, D.C. Hong, and H.E. Stanley, J. Phys. A 17, L261 (1984).
- [22] M.D. Rintoul and H. Nakanishi, J. Phys. A 25, L945 (1992).
- [23] P. Grassberger, J. Phys. A 25, L945 (1992).
- [24] M.D. Rintoul and H. Nakanishi, J. Phys. A 27, 5445 (1994).
- [25] D. Stauffer and A. Aharony, *Introduction to Percolation Theory* (Taylor and Francis, London, 1992).
- [26] B.I. Halperin, S. Feng, and P.N. Sen, Phys. Rev. Lett. 54, 2391 (1985); S. Feng, B.I. Halperin, and P.N. Sen, Phys. Rev. B 35, 197 (1987).
- [27] S. Havlin and D. Ben-Avraham, Adv. Phys. **36**, 695 (1987), and references therein.
- [28] P.M. Lam, J. Phys. A 23, L831 (1990).
- [29] H. Nakanishi, S. Mukherjee, and N.H. Fuchs, Phys. Rev. E 47, R1463 (1993); see also S. Mukherjee, H. Nakanishi, and N.H. Fuchs, *ibid.* 49, 5032 (1994).
- [30] S. B. Lee and H. Nakanishi, J. Phys. A 33, 2943 (2000).