Short-time dynamics of an Ising system on fractal structures

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The short-time critical relaxation of an Ising model on a Sierpinski carpet is investigated using Monte Carlo simulation. We find that when the system is quenched from high temperature to the critical temperature, the evolution of the order parameter and its persistence probability, the susceptibility, and the autocorrelation function all show power-law scaling behavior at the short-time regime. The results suggest that the spatial heterogeneity and the fractal nature of the underlying structure do not influence the scaling behavior of the short-time critical dynamics. The critical temperature, dynamic exponent z, and other equilibrium critical exponents β and ν of the fractal spin system are determined accurately using conventional Monte Carlo simulation algorithms. The mechanism for short-time dynamic scaling is discussed.

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I. INTRODUCTION

The order-disorder phase transitions on structures exhibiting self-similarity have attracted much attention in the past two decades in the research fields of statistical physics and materials science. A typical example is the growth of precipitates and transient phases or atomic clusters, where certain newly formed phases grow into structures with self-similarity. This includes ordering processes in phase separation or solidification [1], liquid-to-glass transition, and condensation or aggregation of nanosized particles. There are some other examples, such as catalytic process on a fractal surface [2,3], reaction diffusion on porous media [4], and spinodal decomposition on a fumed silica network [5], where the underlying structures supporting the processes are most evident in their fractal characteristics. In the growing phase that forms a fractal as well as the physical processes taking place on foreign fractal objects, the influence of the underlying fractal structure on material processing and final properties is significant [1–5]. Therefore, how the fractal structure affects the kinetics of such phase transitions is a fundamental issue that is worthy of serious consideration. To date, however, the exact mechanism is still an open question and its theoretical understanding is very limited [1–3].

Recently, it was found that the ordering process depends on the fractal structure to which the system is confined [5–7]. On a finitely ramified fractal structure such as diffusion-limited aggregated clusters [5] or a Sierpinski gasket [6], the kinetics of domain growth is shown to obey dynamical scaling and universality. On an infinitely ramified fractal structure such as a Sierpinski carpet, dynamical scaling is found to be no longer valid because the growing interface is pinned by the depleted holes of the fractal structure [7]. However, this kinetic mechanism found in the numerical simulations is not consistent with statistical mechanics studies of the phase transition on a fractal structure where the model system, e.g., an Ising model, on an infinitely ramified fractal structure has a well-defined ordered phase below a nonzero critical temperature T_c [8]. This apparent inconsistency in the aforementioned work is the main motivation of this work to understand how the fractal structure influences the dynamic behavior of the transition.

Intuitively, we would expect that near T_c, the system feels the effect of the underlying fractal structure less since the spin-spin correlation length ξ tends to infinity at the late stage of ordering. At the early stage of kinetics when the correlation length ξ is small, we should expect the largest impact of the inhomogeneous fractal structure on the domain growth. As a result, the correlation function should not show dynamical scaling at the early stage. Therefore, the short-time kinetics could serve as a stringent test case for understanding how fractal structure affects phase transitions.

The model system we use in this work is an Ising model at T_c embedded in a Sierpinski carpet. To the best of our knowledge, there has been no work done to investigate the dynamical relaxation at temperature $T \leqslant T_c$ in this model. In this temperature region, the relaxation time of the fractal spin system is known to be extremely long, which imposes a tremendous burden for simulations. As a consequence, neither the T_c nor the dynamic exponent z has been well determined [9]. Our immediate goal, therefore, is to determine these properties. The method we use is the short-time dynamic scaling [10]. The short-time scaling regime was first predicted by Jassen, Schaub, and Schmittmann [10] using the field-theoretic and renormalization-group methods, and was confirmed subsequently by many computer-simulation studies [11–14]. At the critical temperature, the evolution of physical quantities at early times is shown to obey power-law dynamic scaling [10]. For instance, the order parameter, e.g., the magnetization $M(t)$, undergoes a dynamic initial increase at an early time scale,

$$M(t) \sim m_0 t^{\theta} F(t^{\theta+\beta/\nu z} m_0), \tag{1}$$

where $m_0 \equiv M(0)$ is small and θ is a new universal exponent. The scaling function $F(x) \sim 1$ for $x \to 0$ and $F(x) \sim 1/x$ for $x \to \infty$. There is an initial increase at an early (macroscopic) time scale at $t < t_c$, where t_c measures the crossover from the initial growth to the well-known decay relaxation. The positive m_0 leads to the initial growth of the up-spin domain [14], and the correlation function displays the scaling behavior [10,15]

$$C(r,t;\tau) = r^{-D+z\theta} F(r^z/t, r\tau^{\nu}), \tag{2}$$

where $\tau=(T_c-T)/T_c$ and D is the spatial dimension. Although the exact mechanism for such a general mechanism is still not fully emerged, the apparent success of the short-time scaling, as seen in many cases studied by various means [10–15], makes the approach very attractive for our work. Another practical advantage of the short-time dynamics is that we can use the scaling exponents calculated from the short-time regime to determine the equilibrium critical exponents [11,14]. This gives us a convenient way to study the ordering process and critical phenomena in systems with an extremely long relaxation time.

Besides testing the dynamic scaling of the fractal Ising model, another very desirable outcome from this wok, as we discussed earlier, is to see whether or not the short-time scaling [10] works in this special case. The short-time scaling behavior is verified only in the systems in Euclidean space [11–16]. It is not clear if it is still valid on a fractal structure whose critical temperature T_c is nontrivial. In systems without translational invariance, such as a Sierpinski carpet, there are entire length scales of hole space on which no spins can be placed, and therefore the model has no definition. Any finite correlation length is expected to result in the nonuniversal behavior of an initial increase of the order parameter. The same question has been asked for systems with impurities or random defects [15,16].

In this paper, we study the Ising model on a Sierpinski carpet at the critical temperature using extensive Monte Carlo simulations. Our emphasis is on the effect of a fractal structure on the short-time kinetics. The critical temperature, equilibrium exponents, and dynamic exponent will be determined. In Sec. II, the model system and the dynamic short-time scaling relation are introduced. In Sec. III, Monte Carlo simulation results in the fractal systems with various sizes will be presented. In Sec. IV, we discuss the mechanism of short-time scaling on the fractal structures.

II. MODEL AND CRITICAL SHORT-TIME DYNAMICS

A. Ising model on a Sierpinski carpet

We consider a system with N spins $S_i=\pm 1$, which are placed on the vertices of a Sierpinski fractal structure. The Sierpinski carpet is generated with the following procedure: A full square of length L is divided into b^2 equal squares; l squares are chosen out of these squares and removed. In the next iteration, each of the small squares left are divided again into b^2 squares and l of these squares located at the same positions as in the first iteration are removed. The fractal dimension of the remaining area after n iterations is $d=\ln(b^2-l)/\ln(b)$ when the number of iterations n is large. In this work we use the Sierpinski carpet with $b=3$ and $l=1$. As shown in Fig. 1, the hole(s) of the squares at the center are removed in each iteration. It is proven that when $n\geqslant 6$ $(L\geqslant 2187)$, the topology of this fractal is determined and the effect of the boundary condition can be neglected [17].

The Hamiltonian of the system is written as [8]

$$\hat{H}=-\sum_{\alpha} J_{\alpha}\sum_{\langle i,j\rangle} S_i S_j, \tag{3}$$

where $\langle i,j\rangle$ denotes the sum extending over all nearest-neighbor spins. $J_{\alpha}(>0)$ is the coupling constant between two nearest-neighbor spin. $J_{\alpha}=J$ if the bond is common to two iterative elementary squares. If the edge is a wall of a noniterative area, we set $J_{\alpha}=J_w$, where $J_w\neq J$. Since we are interested only in the effect of a fractal structure on short-time dynamics, and the heterogeneity in J_{α} as presented by the different J's may come into effect [16], we set $J_{\alpha}=J_w=J$ in this work. T is temperature in units of J/k_B.

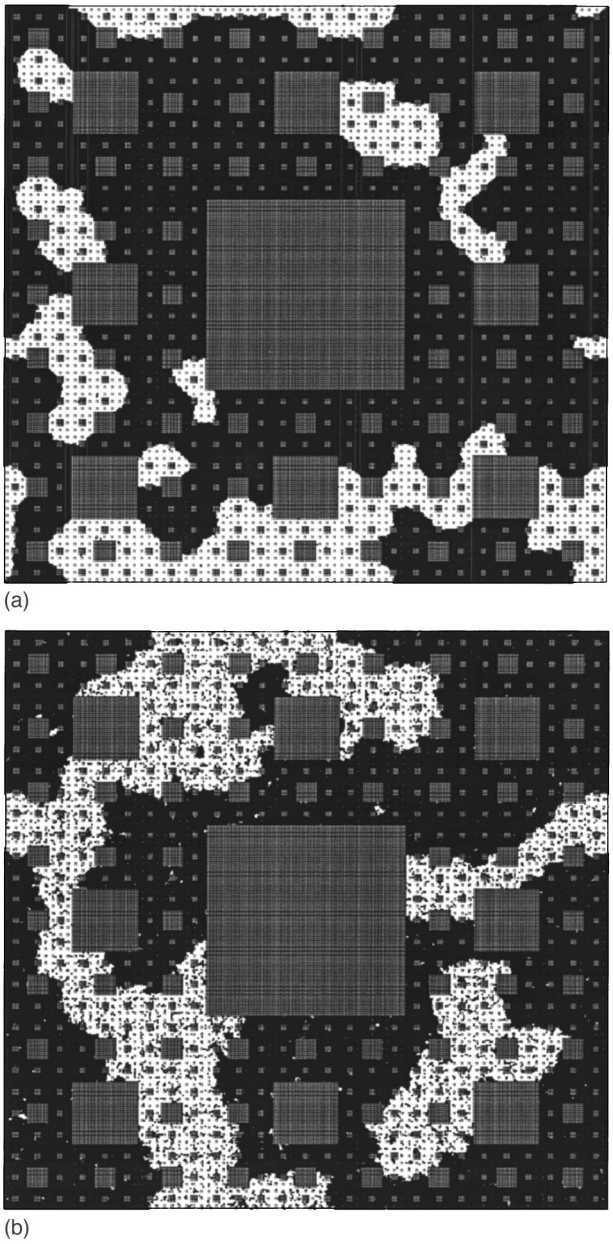

FIG. 1. Domain structures of the Ising model embedded on the Sierpinski carpet after the quench to temperature: (a) $T=T_c/2$, (b) $T=0.9T_c$. The system size is $L=729$. The up (down) spins are denoted by black (white). The depleted area of the Sierpinski carpet is in patterned gray. $m_0=0$, $t=100\,000$ MCS.

The model described by Eq. (3) is solved in Ref. [8] using the Migdal-Kadanoff renormalization-group technique, and the critical temperature and exponents are calculated *approximately*. The dynamic exponent z is also determined by the dynamical renormalization-group method [9]. The Monte Carlo simulation and the ε expansion were used for this model system [17–21].

There are some difficulties in the Monte Carlo simulation in calculating the critical temperature and critical exponents. The first, and the most important, is a critical slowing down. The relaxation time of a fractal system is much larger than that of a Euclidean system. Due to limited simulation time, it is difficult to get accurate results for fractal spin systems using the conventional Monte Carlo simulation. Second, although the cluster algorithms can improve the efficiency of the Monte Carlo simulation considerably for large systems [17,18], it may not be applicable to the systems that obey Glauber dynamics. The finite-size scaling for the cluster algorithms may exhibit behavior inconsistent with that following the Glauber dynamics [22]. Third, the dynamic exponent z, which is an essential quantity for the kinetic process, could not be accurately determined. As a result, z has not been well determined in a fractal system by both simulations [18,21] and the renormalization-group method [9]. In this paper, we study the critical dynamics of this model system in the short-time regime in order to avoid the critical slowing down. As we show later, dynamic critical phenomena can be studied using the conventional Monte Carlo method in the short-time regime, and as a result the wanted critical temperature and critical exponents can be determined accurately.

B. Universal scaling for critical relaxation

When an Ising system is quenched from high temperature to its critical temperature T_c, it is well known that the order parameter $M(t)$ decays to zero by a power law [14], $M(t) \sim t^{-\beta/\nu z}$, at late times. The relaxation time $t_0 \sim L^z$ becomes infinite as $L \to \infty$. Therefore, strictly speaking, this kind of critical relaxation can never be observed in numerical simulations. In the past decade, new critical kinetics was discovered for the critical quench, and the corresponding new dynamic exponents which are independent of β, ν, and z were introduced. In the following, we briefly describe the short-time dynamics and the critical exponents.

Short-time dynamics [11]

The kth moment of magnetization has the scaling relation

$$M^{(k)}(t,L;\tau,m_0) = b^{k\beta/\nu} M^{(k)}(b^z t, bL; b^{-1/\nu}\tau, b^{-x0} m_0), \tag{4}$$

where b is the scaling factor of the system size. $m_0 = M(0)$ and x_0 measures its dimension. When quenched from disordered states ($m_0 = 0$), in a large system and short time, Eq. (4) yields the following power-law scaling relations:

$$\langle M(t)\rangle \equiv \left\langle \frac{1}{N}\sum_{i=1}^{N} S_i \right\rangle \sim t^{\theta}, \tag{5a}$$

$$\chi(t) = \langle M^2(t)\rangle \equiv \left\langle \left(\frac{1}{N}\sum_{i=1}^{N} S_i \right)^2 \right\rangle \sim t^{[d-2\beta/\nu]/z}, \tag{5b}$$

and

$$\langle C(t)\rangle \equiv \left\langle \frac{1}{N}\sum_{i=1}^{N} S_i(t) S_i(0) \right\rangle \sim t^{d/z-\theta}. \tag{5c}$$

Here $\langle\ \rangle$ denotes the average over the replica of initial states. θ is a new dynamic exponent that characterizes the short-time evolution and β,ν are equilibrium critical exponents. If the system evolves from a totally ordered state ($m_0 = 1$), the following equations hold:

$$\langle M(t)\rangle \sim t^{-\beta/\nu z}, \tag{5d}$$

$$\frac{\partial}{\partial \tau}[\ln\langle M(t)\rangle]_{\tau=0} \sim t^{1/\nu z}, \tag{5e}$$

and

$$U(t) \equiv \frac{\langle M^2(t)\rangle}{\langle M(t)\rangle^2} - 1 \sim t^{d/z}. \tag{5f}$$

Equations (5) are valid before the evolution changes to the late-time relaxation kinetics. Using the dynamic scaling relations (5a)–(5f), the critical temperature and the exponents can be determined at the short-time regime, so that computing time can be dramatically reduced.

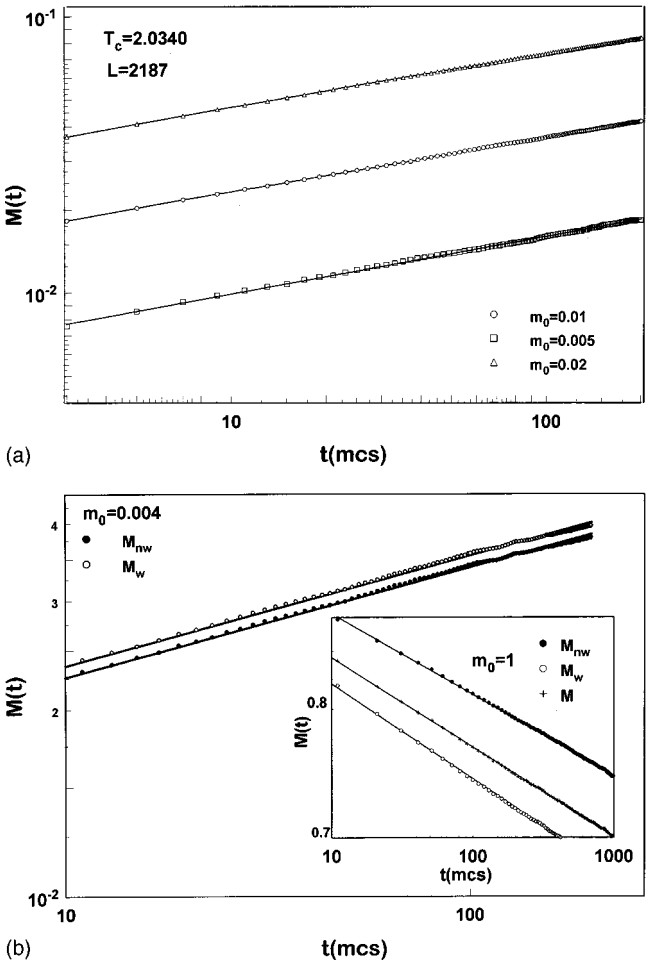

FIG. 2. (a) The log-log plot of the total magnetization at early times at critical temperature after quenching from initial magnetization m_0. The system size is $L = 2187$. The solid lines are the fits to power-law curves. (b) The evolution of magnetization M_w and M_{nw} in log-log scale. $m_0 = 0.004$. The inset shows those when $m_0 = 1$. $L = 2187$ and $T = T_c$. The solid lines are the fits to the power law.

TABLE I. The scaling exponent θ for initial slip.

m_0	0.02	0.01	0.004
$L=729$	0.167	0.173	0.186
$L=2187$	0.188	0.196	0.205

Persistence probability of critical quench

The probability $p(t)$ that the global order parameter has not changed sign in time t following a quench to the critical temperature was found to obey the power-law scaling in a nonconserved $O(N)$ model in the large-N limit and the Ising model using the Monte Carlo simulation [23],

$$p(t)\sim t^{-\theta'}, \tag{6}$$

where θ' is another new nontrivial exponent for the critical dynamics.

III. Monte Carlo simulation studies

The Monte Carlo simulation was carried out in the system described by Hamiltonian (3). Periodic boundary conditions are used. As discussed in Sec. II, the boundary condition did not affect the fractal nature of the system when the system size was large. The initial configuration of the system is prepared with a definite m_0. The update of each spin is carried out using the heat-bath algorithm. An attempt to update all spins is defined to be one Monte Carlo step (MCS). Physical quantities are measured at time t and are averaged over samples with different initial configurations while m_0 is kept constant. As a comparison, we also used the Metropolis algorithm for updating spins. The results were found to be the same at the time scale $t>t_s$. t_s is typically 10 MCS. Therefore, the following calculation was based on the data at $t>t_s$.

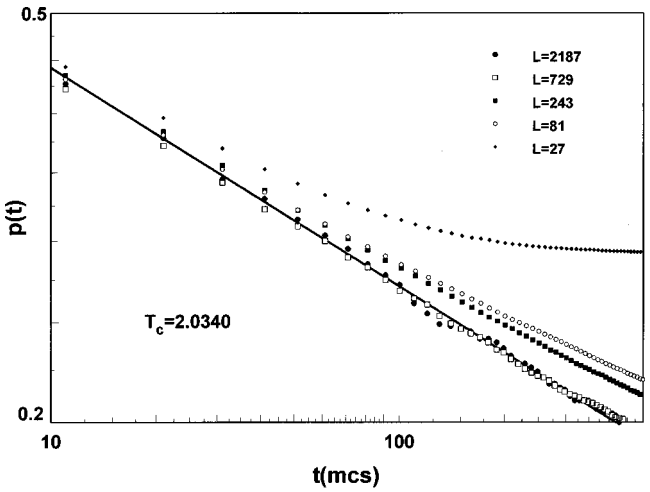

FIG. 3. Log-log plots of the persistence probability of spins after being quenched to T_c. $m_0=0$. The solid line is the fits to the power law. Finite-size effect is shown.

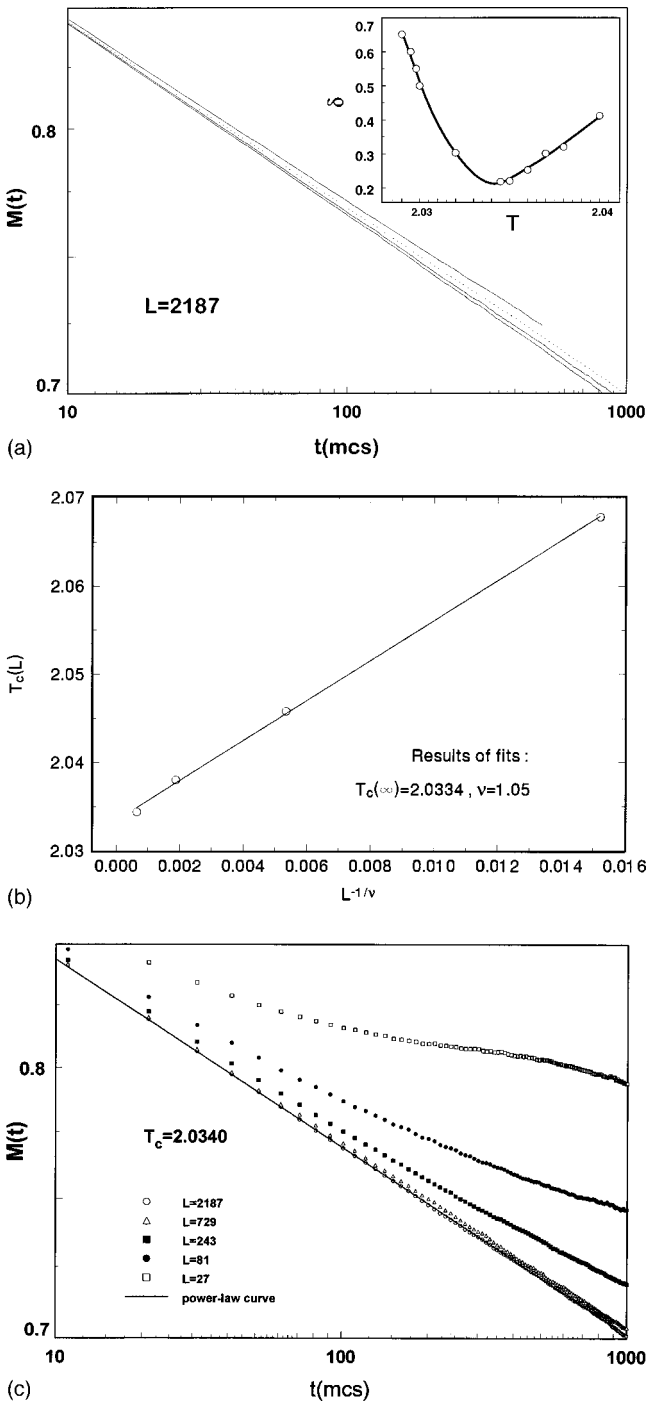

FIG. 4. (a) Log-log plots of the evolution of total magnetization from an initial ordered state ($m_0=1$) at $T=2.032$, 2.036, and 2.037 (from above, solid lines). The dashed line is that at $T_c=2.0344$, which is determined by finding the minimum square derivation from power-law fits, as shown in the inset. (b) Finite-size scaling for the critical temperature $T_c(L)$ (open circles). The solid line is the best fit to Eq. (7). (c) Finite-size effect on the magnetization at T_c ($m_0=1$). The solid line is that at $T_c(\infty)=2.0334$. The plots are in log-log scale.

A. Critical initial slip and persistence probability

Figure 2 shows the initial increase of magnetization from different m_0 at $T_c=2.03$. We have checked the finite-size effect on the evolution and found that it diminishes as $L>729$.

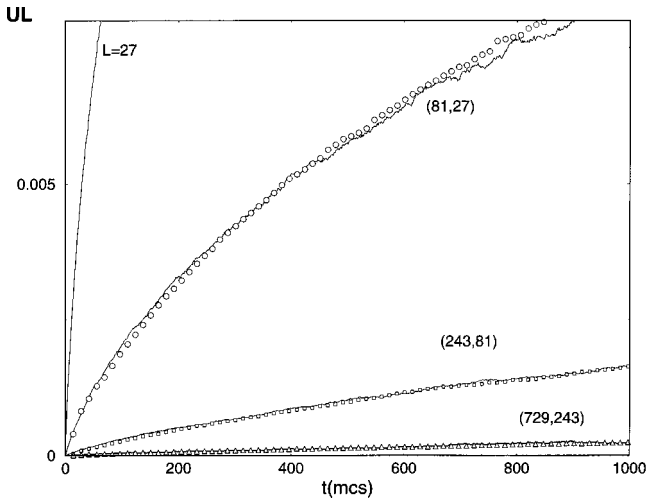

FIG. 5. The scaling of Binder cumulant *UL* for a pair of lattices (L_1,L_2). The solid lines are *UL* for systems in size L_1, the open symbols are those for systems in size L_2. The time is rescaled by the factor of $(L_2/L_1)^z$. The system evolves from $m_0=1$ at T_c.

The magnetization of the fractal Ising system is found to be inhomogeneous. We consider two regions on the carpet and calculate their mean magnetizations: $M_w=(\Sigma\sigma_i)/N_w$ and $M_{nw}=(\Sigma\mu_i)/N_{nw}$. Here σ_i are the spins on the internal walls bordering the eliminated areas and N_w is the total number of these spins. μ_i are the spins that are not on the internal walls and $N_{nw}=N-N_w$ is the number of them. The equilibrium critical exponents for M_w and M_{nw} are found to be different [24]. Figure 2(b) shows M_w and M_{nw}. We can see that as $m_0\to 0$, the evolution of $M(t)$, $M_w(t)$, and $M_{nw}(t)$ increases with the power law in time. The exponents can be determined by linear extrapolation to $m_0=0$, and the exponents are nearly the same. Table I lists the results from the fitting. It is interesting to see that the fractal structure does not affect the exponent θ, and short-time dynamic scaling is universal for an Ising system on a fractal structure. It seems that this kinetics of initial slip is not the same as the evolution of the system that starts from an ordered state $(m_0=1)$, which follows Eq. (5d). As shown in the inset of Fig. 2(b), the difference in exponents is found for $M(t)$, $M_w(t)$, and $M_{nw}(t)$.

The persistence probability $p(t)$ of the magnetization of the system is shown in Fig. 3. The evolution is found to follow Eq. (6) as $L>729$ with the persistence exponent $\theta'=0.210(7)$.

B. Critical temperature determined by short-time dynamics

At critical temperature, when the system decays from an order state $(m_0=1)$, the magnetization follows a power-law scaling relation described by Eq. (5d). This scaling behavior can be used to determine T_c $(L=\infty)$ in the thermodynamic limit by finding the critical temperature of the finite-size system $T_c(L)$ at which the decay follows the power law. Figure 4(a) shows the decay of magnetization at different temperatures. For a system with length L, $T_c(L)$ is calculated by finding the smallest error of the power-law fit for $M(t)$, as shown in the inset in Fig. 4. The critical temperature is then determined by finite-size scaling,

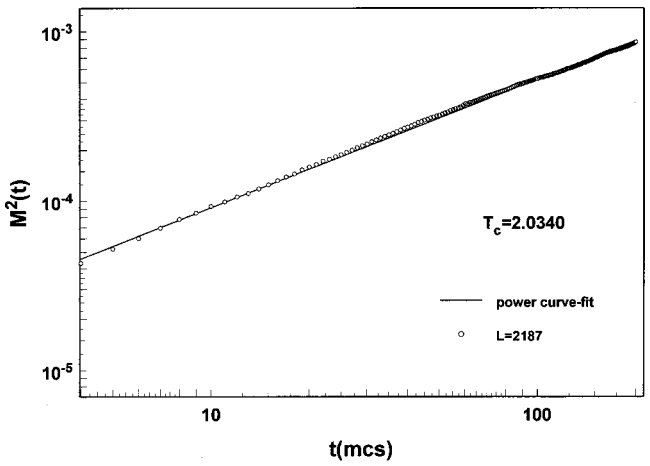

FIG. 6. Log-log plot of the second moment of magnetization at T_c. The system started from $m_0=0$.

$$T_c(L)-T_c(\infty)\sim L^{-1/\nu}. \tag{7}$$

Figure 4(b) shows the scaling relation. The critical temperature for this system is found to be $T_c(\infty)=2.0334\pm 0.0005$. This value agrees with the equilibrium Monte Carlo simulation result $T_c=2.03$ [20], but with higher accuracy. Figure 4(c) shows the finite-size scaling for $M(t)$ at $T_c(\infty)$ using the relation Eq. (4) with $m_0=1$. Corresponding exponents β/ν and z can also be determined. Equation (4) together with Eq. (7) can be used to calculate $T_c(\infty)$, β, ν, and z self-consistently with high accuracy.

C. Dynamic critical exponent z determined by finite-size scaling

Once T_c is found, the dynamic critical exponent can be determined by finite-size scaling from the Binder cumulant. At $T_c(\infty)$, the cumulant of magnetization follows the scaling relation

$$U(t,L_1)=U(tb^z,L_2), \tag{8}$$

where $b=L_2/L_1$. Figure 5 shows the data collapse of

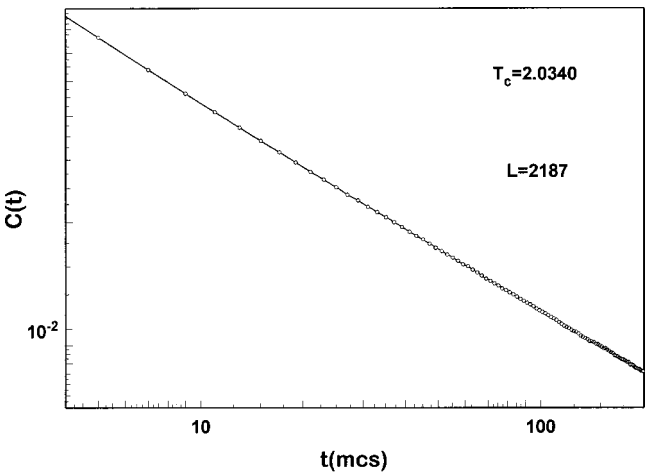

FIG. 7. Log-log plot of the autocorrelation function at T_c. The system started from $m_0=0$.

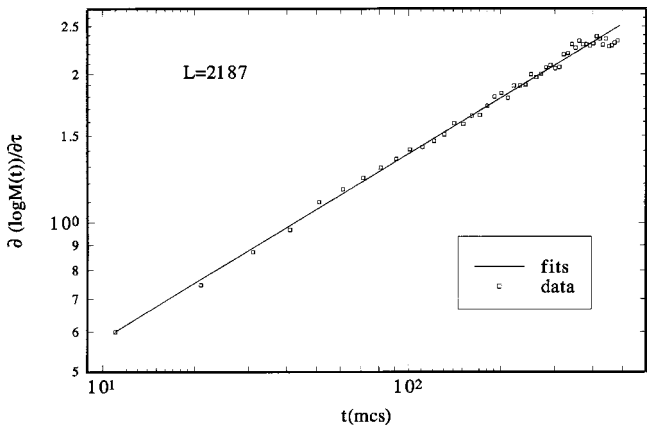

FIG. 8. Log-log plot of the derivative of $\ln(M(t))$ to the reduced temperature τ. The open boxes are calculated by extrapolation to $\tau=0$. The solid line is the power-law fits at $T=T_c$. The system started from $m_0=1$.

$U(t,L)$. The average value of the dynamic critical exponent is $z=2.38(4)$.

z can also be calculated from the finite-size scaling of persistence probability $p(t)$ [23], $p(t)=L^{-\theta' z}F(t/L^z)$, as shown in Fig. 3. The result is consistent with that determined by Eq. (8). It is interesting to find that $\theta' z$ is the same as that in a pure Ising model [23].

D. Equilibrium exponents

The equilibrium exponents β,ν can be determined by using the scaling relations (3b)–(3e). Figure 6 shows the second moment of magnetization and Fig. 7 shows the autocorrelation function. The system evolves from the initial state $m_0=0$. Figure 8 shows the first derivative of $M(t)$ curves in Fig. 4(b) with respect to the reduced temperature, which is fitted to Eq. (5e).

We found that the values of β and ν agree well with the values calculated by finite-size scaling, as mentioned in Secs. III A–III C. We list all the exponents computed in this work in Table II. For comparison, the corresponding exponents determined by other methods are also tabulated.

IV. DISCUSSION

Our simulation results show that the Ising system on a Sierpinski carpet follows the dynamic scaling at short times after it is quenched to the critical temperature. The fractal nature, as represented by all length scales of internal holes, does not affect the power-law dynamic scaling in the short-time regime. In the time scale of typically 1000 MCS, the correlation length ξ for spins is not larger than 50. But the mean magnetization of all spins on the internal walls shows universal power-law behavior. This indicates that the structural heterogeneity does not affect the kinetics; and scaling exponents for the two regions are the same. Therefore, the dynamic scaling relation (2) may still be valid in the Ising model embedded on an infinitely ramified fractal structure.

TABLE II. Critical temperature T_c and critical exponenets determined by different methods: (a) renormalization-group method [16] (an asterisk denotes $J_w=0$ using the dynamic renormalization-group method [18]), (b) Monte Carlo simulation [21], (c) short-time dynamic scaling, and (d) pure Ising model [10,25].

	T_c	β	ν	z	θ	$\theta' z$
(a)	3.11		1.12	3.915*		
(b)	2.03 ± 0.02	0.0928	1.09	2.20 ± 0.06		
(c)	2.033(4)	0.102(4)	1.05(4)	2.38(4)	0.211(3)	0.502(7)
(d)	2.269	0.125	1	2.155	0.191	0.505

In addition, our results show that the initial ordering of the system is not a *local* event. If the increase of magnetization is due to local domain growth in short time and the thermal fluctuation is not relevant, as pointed out in Ref. [14], the short-time scaling regime will be very small (less than 10 Monte Carlo steps) in the system we studied. If there is no activation of local spin clusters, the domain wall will be pinned by the internal holes. This phenomenon can be seen in Fig. 1.

In heterogeneous systems such as the spin systems in which the interactions among spins are not homogeneous, the validity of the critical short-time dynamics is questionable [15,16,25]. However, in the system without translational invariance, we demonstrated in our simulations that short-time dynamics [Eq. (5)] is valid. Based on our simulation results, the theoretical explanation for short-time dynamics proposed in Ref. [14] may need to be reconsidered. This calls for further investigation on the underlying physics of short-time dynamics.

V. CONCLUSION

We have studied the critical short-time dynamics of an Ising system on a Sierpinski carpet. Dynamic scaling is found for the short-time evolution and the critical exponents are measured. Using short-time dynamic scaling, we are able to determine the critical temperature and the dynamic critical and equilibrium exponents. The results are in fairly good agreement with those calculated by equilibrium techniques but with higher accuracy.

ACKNOWLEDGMENTS

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