

Molecular-dynamics simulations of quenched two-dimensional anisotropic XY models

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In this paper results of molecular-dynamics simulations of a quenched anisotropic XY model are presented. At late stages an algebraic growth law satisfying the classical Lifshitz-Allen-Cahn law has been found. Thus the results in the present paper are in agreement with the results found in Monte Carlo simulations, hence suggesting that the Monte Carlo time measure is related linearly to real time at late stages. Furthermore, at early stages an exponential growth of the ordered states has been found—in agreement with the linearized Cahn-Hilliard equation.

I. INTRODUCTION

The domain-growth kinetics of two-dimensional Potts and Ising models as well as two-dimensional continuous-rotor or XY models has been studied in the literature by Monte Carlo simulations. The asymptotic growth law of the average linear extension of the domains as a function of time is usually described as

$$l(t) \approx at^n \quad (1)$$

where n is referred to as the growth exponent.

In Refs. 1–3 the growth laws for Potts and Ising models have been studied, and Eq. (1) has been found to hold with exponent value $n = \frac{1}{3}$ for conserved order parameter, and $n = \frac{1}{2}$ for nonconserved order parameter, where the latter also is the result of the classical Lifshitz-Allen-Cahn theories.^{4,5} From Monte Carlo simulations of continuous single-site rotor or XY models^{6–10} the Lifshitz-Allen-Cahn value $n = \frac{1}{2}$ has also been established.

The validity of the measurements of the growth exponents by Monte Carlo simulations is uncertain due to the lack of a convincing argument that the time measure of Monte Carlo simulations is related linearly to real time. In molecular-dynamics simulations the real time is obtained directly, and thus a molecular-dynamics simulation of a growth process would be useful to establish whether the Monte Carlo time is linear or not. There have been some studies of quenching using molecular dynamics on Lennard-Jones liquids.^{14–16} However, they studied phase separation cluster growth, where the growth exponent is explained through a Lifshitz-Slyozov-like analysis. Thus there seem to be no molecular-dynamics studies of quenched Lifshitz-Allen-Cahn-type models available.

In this paper simulations for the growth exponent of the classical $p=2$ XY model studied by the Monte Carlo method in Ref. 10 are repeated, but using the molecular-dynamics method instead. The aim of the present paper is to check whether an $n = \frac{1}{2}$ exponent is found at finite temperatures. In Sec. II the model is presented, and the molecular-dynamics method necessary to simulate a constant temperature system is discussed. In Sec. III the computational details and results of the simulations are

presented. It is found that the $n = \frac{1}{2}$ dependence at finite temperatures indeed holds. At early times an exponential growth of the ordered states has been found. This is in agreement with the classical linearization of the Cahn-Hilliard equation.¹⁷

II. THE MODEL AND THE SIMULATION METHOD

A classical twofold degenerate XY-spin model is used. The corresponding Hamiltonian is

$$H = \frac{1}{2} \sum_i \dot{\phi}_i^2 + \frac{1}{2} J \sum_i \sum_{j \in (NNN)^i} \cos(\phi_i - \phi_j) - \frac{1}{2} P \sum_i \sum_{j \in (NN^i)_x} \cos(\phi_i) \cos(\phi_j), \quad (2)$$

where $J > 0$, $P > 0$ and $(NNN)^i$ indicates that the sum is on next-nearest neighbors to rotator i only, whereas $(NN^i)_x$ indicates a sum over nearest neighbors in the x direction. In an ordered domain neighbors in the x direction are aligned with the same direction, whereas neighbors in the y direction are aligned with opposite directions. Thus the two degenerate ordered domains are antiferromagnetic. This Hamiltonian has been used in Ref. 10 to find the growth exponent by Monte Carlo simulations. In the classical method of molecular dynamics, the equations of motion are derived directly from Eq. (2):

$$\ddot{\phi}_i = J \sum_{j \in (NNN)^i} \sin(\phi_i - \phi_j) - P \sum_{j \in (NN^i)_x} \sin(\phi_i) \cos(\phi_j). \quad (3)$$

In thermodynamical equilibrium this method produces trajectories corresponding to the microcanonical ensemble. A molecular-dynamics simulation of a quenched dynamical system using this method thus has the serious drawback that it will not converge to the true canonical ensemble dynamics as time goes to infinity. Moreover, the intermediate distributions conserve the total energy obtained at zero time, which yields instantaneous temperatures of the system, which are too high. A modification of the method is needed that simulates the system in exchange with a heat bath at fixed temperature, still allow-

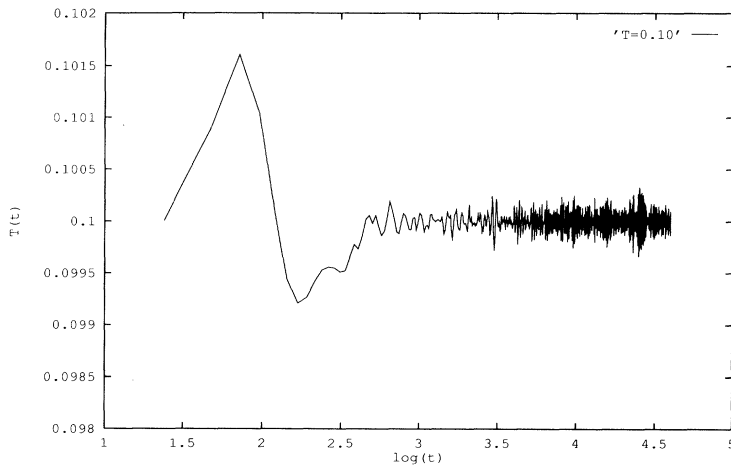


FIG. 1. Instantaneous temperature as a function of time.

ing fluctuations of the instantaneous temperature in the system. Nose^{11,12} found a solution to this problem. He constructed an extended Hamiltonian, which he proved to yield statistics of the canonical ensemble at thermodynamical equilibrium. The method was simplified by Hoover.¹³ Applying Hoover's simplification yields the following (Nose-Hoover) equations of motion:

$$\begin{aligned} \ddot{\phi}_i &= J \sum_{j \in (NNN^i)} \sin(\phi_i - \phi_j) \\ &\quad - P \sum_{j \in (NN^i)_x} \sin(\phi_i) \cos(\phi_j) - \psi \dot{\phi}_i, \\ \dot{\psi} &= \sum_i (\dot{\phi}_i^2 - NkT) / Q, \end{aligned} \quad (4)$$

where N is the total number of rotators, T is the temperature of the external heat bath, and $Q > 0$ is an arbitrary constant. The value of Q should be chosen carefully to yield good statistics of the simulations.¹¹ Notice that this is the real time formulation of the Nose-Hoover equations. This is important since time scaling should be avoided.

A quench from a high temperature T_h to a quench

temperature T_q could thus be simulated using the Nose-Hoover equations in the following way: (1) Equilibrate the system using the Nose-Hoover equations at $T = T_h$; (2) change the value of T to T_q ; (3) simulate the quench using the Nose-Hoover equations at $T = T_q$.

Notice that the additional variable ψ influences the system in a harmonic manner allowing oscillations of the instantaneous temperature about the equilibrium temperature T . When the method is applied to a system which is started off at an instantaneous temperature far away from T , the oscillations are damped rather slowly. This causes a rather serious drawback in a study of the early stage ordering dynamics using the method above, since the oscillations force the instantaneous temperature to drop far below T , which is a rather unphysical effect of the method. Although this effect should cause negligible damage at late stages, the following method is applied instead: (1) Set up a random configuration; (2) Set up random velocities according to T_q ; (3) Simulate the quench using the Nose-Hoover equations at $T = T_q$.

Thus the initial configuration corresponds to an infinite temperature and the instantaneous temperature at zero time is close to T_q . The amplitude of the oscillations of

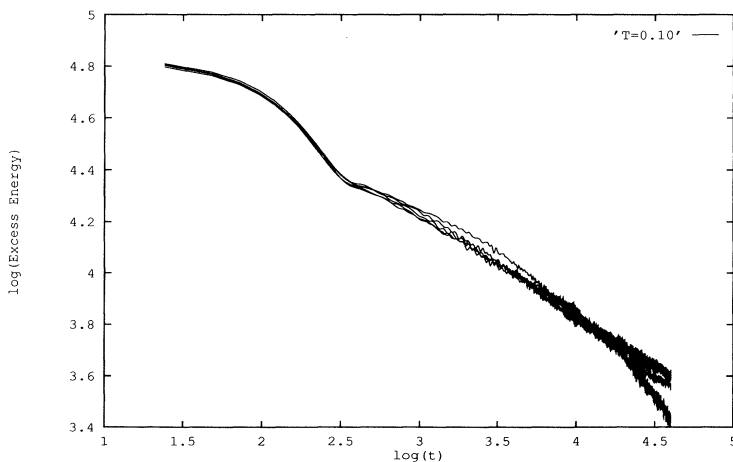


FIG. 2. Log-log plot of the excess energy as a function of time for five different quenches at $T = 0.05$.

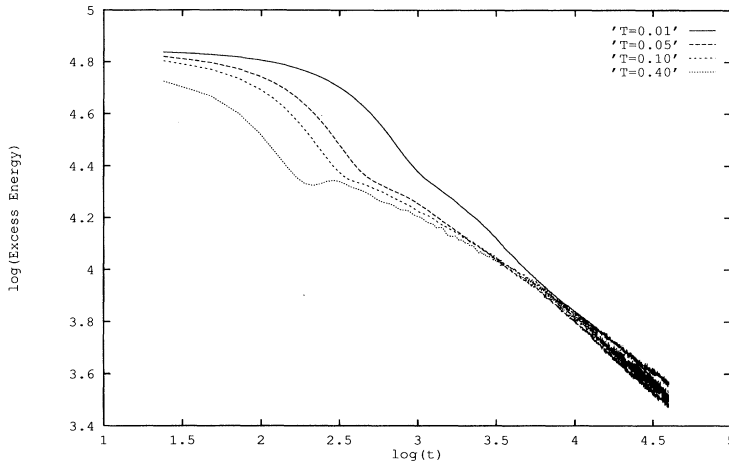


FIG. 3. Log-log plot of the excess energy as a function of time obtained from the average of five different quenches at each temperature.

the instantaneous temperature is therefore small even at early stages.

III. SIMULATIONS AND RESULTS

The model described in the preceding section where $J=1$ and $P=5$ has been simulated using Nose-Hoover molecular dynamics at four different temperatures. The simulations were performed on a grid of 72×72 rotators, and the Nose-Hoover parameter Q was set to 5. The equations of motion were integrated by a fourth-order Runge-Kutta scheme with a stepwise of 0.008, and the simulations were run for 25 000 timesteps on a T800 transputer-based MEIKO computer.

In Fig. 1 the instantaneous temperature is shown as a function of time at a quench to $T=0.1$. The instantaneous temperature reaches equilibrium very fast as expected. (On all figures the time is measured in units of time steps, and the temperature is measured in units of the critical temperature.)

A well-known way (see, for example, Ref. 18) of finding a measure for the average domain size $l(t)$ at time t in a quench at temperature T is by calculating the excess energy:

$$\Delta E(t) = E(t) - E_{eq}(T) = l^{-1}(t). \quad (5)$$

Thus the growth exponent n can be found from the slope of a log-log plot of $\Delta E(t)$. Figure 2 shows a log-log plot of the decay in excess energies from five different quenches at $T=0.1$. It can be seen that the excess energy yields a measure of the growth, which suppresses noise very well. Another way of finding a measure is by using the structure factor. The structure factor was measured, but the results for the average domain size obtained from the structure factor were found to be extremely sensitive to noise compared to the excess energy method. Although moments of the structure factor may be used to suppress the noise, throughout this paper domain sizes are measured using Eq. (5).

In Fig. 3, a log-log plot of the average growth at different temperatures is shown. Different phases of the growth can be obtained from the figure. At early stages, $[\log(t) < 2.5]$, domains are formed by thermalization from a random configuration. At times $[2.5 < \log(t) < 3.0]$ the system changes towards the late stage curvature driven growth ($3.0 < t$), where different domains “compete” with each other.

In Fig. 4 snapshots of the different phases in the growth at $T=0.1$ are shown. In these figures a spin is assumed to belong to a wall if its angle deviates more than $\pi/15$ from a ground state angle. The first two figures in Fig. 4 show the development of the system in the early stage. In the third figure the system is undergoing the crossover to late stage growth. In the fourth figure a very late stage of the system is shown.

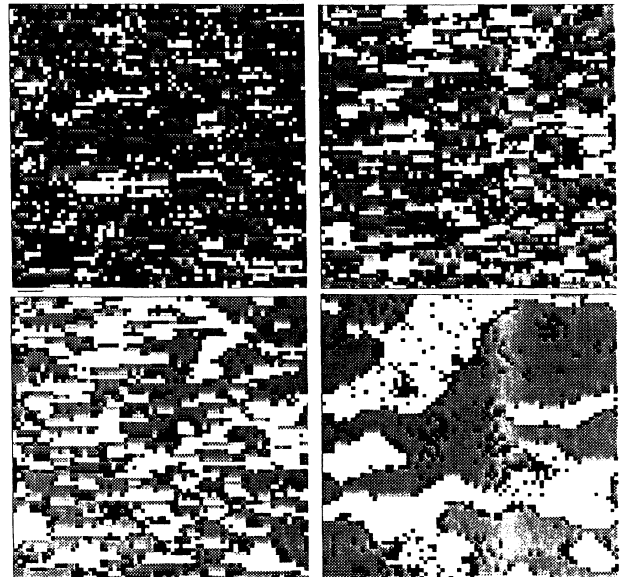


FIG. 4. Snapshots of configuration at different times. Black areas correspond to walls, whereas white and grey areas correspond to the two different domains.

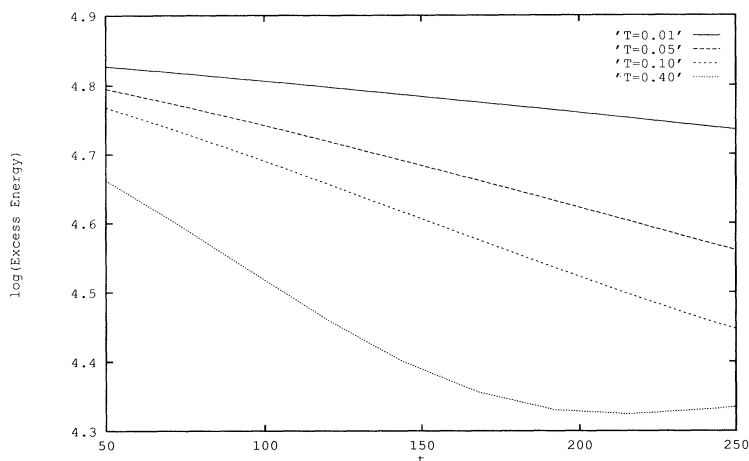


FIG. 5. Log plot of early stage average excess energy as a function of time.

We first study the early stage growth. At zero time the slope of the excess energy curve should be zero due to the fact that the system is started off with random velocities. At early times the system is not subject to domain growth, but it is subject to a growth in size of the order parameter. The linearized Cahn-Hilliard equation¹⁷ predicts that the order parameter grows exponentially at early times. The growth of the order parameter can be measured by the inverse excess energy. In Fig. 5 we see that the decay in the excess energy indeed seems to be exponential during this phase. Furthermore, it can be seen from Figs. 3 and 5 that the rate of growth of the order parameter is temperature dependent. The $T=0.4$ quench decays very fast, which yields a very sharp crossover to the late state phase. At the other end the $T=0.01$ quench decays very slowly, and the crossover is very smooth. Thus the bulk phase of the $T=0.01$ quench is still undergoing thermalization when the late state phase has started.

We now turn to the late stage growth. The growth exponent is found from the slope at late stages. In Fig. 6 the late stage growth is highlighted. It is strongly indicated that the late stage growth is independent of the temperature even in the zero temperature limit. Further-

more, the average slope of the individual curves yields results that are in very good agreement with the Lifshitz-Allen-Cahn law characterized by $n = \frac{1}{2}$. This result is in agreement with the results found from Monte Carlo experiments, and thus the Monte Carlo time is linearly related to the (real) molecular-dynamics time. The oscillations of the individual curves are due to thermal fluctuations primarily from the bulk phases of the system.

IV. DISCUSSION AND CONCLUSION

From the results of the preceding sections it is clear that the method of molecular dynamics is a very good tool for studying quenches. Although only one model has been studied, the universal nature of domain growth indicates that the method can be applied to any other (continuous) Lifshitz-Allen-Cahn model with the same successful result.

At early times it was shown that the system obeys the linearized Cahn-Hilliard equation. This result has not been established from Monte Carlo experiments because of the different type of early time dynamics.

At late stages it was found that the growth exponent found in literature by Monte Carlo methods is in agreement with the growth exponent found in this paper using

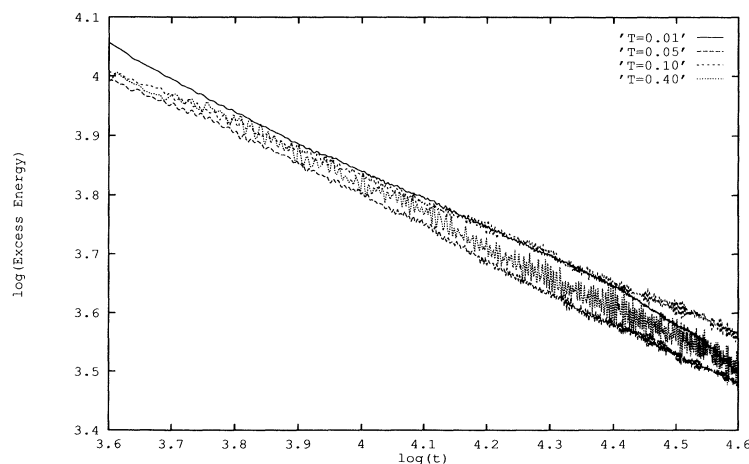


FIG. 6. Log-log plot of late stage average excess energy as a function of time at different temperatures.

the method of molecular dynamics, and thus that the Monte Carlo time is in linear correspondence with real time. In the zero temperature limit, however, there has been found a crossover to a second universality class in Monte Carlo experiments.¹⁰ This universality class is characterized by a growth exponent of $\frac{1}{4}$, and has not been found here. The reason may be that the late stage dynamical behavior is essentially different in the two methods at very small temperatures, and thus that the time measure may become different.

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