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## Domain growth controlled by interfacial transport in two-dimensional systems

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Domain growth is studied for a conserved order parameter when the interfacial particle current dominates the material transport in a two-dimensional system. A simple geometrical model suggests that the typical domain size increases as  $t^{1/4}$  for long times. This behavior is supported by Monte Carlo simulations performed in a half-filled lattice gas taking the first- and second-neighbor jumps and interactions into consideration. [S1063-651X(98)12105-0]

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Domain growth is widely studied in systems of particles with an attractive interaction when the system is quenched from the homogeneous high-temperature phase into the two-phase coexistence region [1]. For a conserved number of particles the initial spatial inhomogeneities evolve into macroscopic domains of high- and low-density phases. Assuming a low initial concentration Lifshitz and Slyozov [2] have shown that the average size of widely spaced particle droplets increases as  $t^{1/3}$  for long times. In this case the growth is limited by a diffusion current from the shrinking droplets to the growing ones through the matrix. The evaporation of the smaller droplets and the growth by condensation of the larger ones are maintained by the Gibbs-Thomson boundary condition at the surface of a spherical droplet.

The situation is different for the half-filled (critical) systems where one can observe connected domains of a complicated and random geometry. Experimental, numerical, and analytical approaches have demonstrated that the system evolves into a scaling regime for sufficiently long times when the domain patterns look statistically similar to those at earlier times. This domain structure is usually characterized by an average linear domain size  $R(t) \sim t^n$ . Analyzing the time-dependent Ginzburg-Landau (TDGL) model for a conserved order parameter, Mazenko [3] has shown that in the early stage of domain coarsening the process is controlled by interfacial diffusion, which gives a  $t^{1/4}$  growth law. Later, however, the bulk diffusion will dominate the growth and results in a faster growth law  $R(t) \sim t^{1/3}$ .

Recent Monte Carlo (MC) simulations of Ising systems [4] and numerical studies of TDGL models [6–8] have confirmed that the classical value of  $1/3$  for the exponent is correct at long times. More precisely, the power-law ansatz for the growth at intermediate times leads to an “effective exponent” of  $n_{eff}(t)$ , which is found to increase continuously with time toward the value  $n=1/3$ . Generalizing the Lifshitz-Slyozov theory, Huse [9] has suggested that the time dependence of the effective exponent be given as

$$n_{eff} = n - C/R(t), \quad (1)$$

where  $n=1/3$  and  $C$  is related to the enhanced interfacial conductivity. This result is supported by evidence from some computer simulations [9,4,6]. Using the so-called cell dynamical system approach, Puri and Oono have indicated a crossover behavior from the earlier exponent of  $n \approx 1/4$  to the asymptotic value [7]. A similar transient was observed by Roland and Grant [5] when studying the two-dimensional Ising ferromagnet with a spin-exchange mechanism.

In the present work our investigation will concentrate on two-dimensional systems where the role of bulk diffusion is negligible. Adapting a geometrical approach, it will be shown that the interfacial transport itself leads to  $n=1/4$  in the scaling regime. This process will be demonstrated by MC simulations in a lattice-gas model that clearly exhibits the  $n \approx 1/4$  behavior in a wide time regime.

The geometrical model of interface evolution was introduced by Brower *et al.* [10] to study the kinematics of moving boundaries appearing for dendritic solidification. During the investigated processes the extension of the interface increased with time as a result of interfacial instability. Now the opposite case will be studied. The geometrical approach will be described briefly because many details of the calculations are given in previous papers [10–12].

In this approach the domain structure is characterized by a set of (nonintersecting and differentiable) closed curves specified parametrically by the position vectors  $\mathbf{x}_\alpha(t, s)$  separating the two phases where  $s$  denotes the arclength. First we concentrate on a single curve neglecting its index  $\alpha$  where it is possible.

In the isotropic system we assume that the projection of the velocity in the normal direction ( $v_n$ ) depends on the local curvature  $\kappa(s, t)$  and on its derivatives with respect to the arclength, namely,

$$v_n = U(\kappa, \partial_s \kappa, \dots). \quad (2)$$

In this case the equation of motion for the curvature obeys the simple form

$$\dot{\kappa} = - \left[ \kappa^2 + \frac{\partial^2}{\partial s^2} \right] U. \quad (3)$$

This equation of motion involves a nonlocal contribution at fixed  $s$  because  $\dot{\kappa}(s,t) = \partial \kappa / \partial t + \dot{s} \partial \kappa / \partial s$  [10–12].

The function  $U$  is determined by assuming that the material transport along the interface is driven by the derivative of the chemical potential  $\mu$  with respect to  $s$ , while  $\mu$  is proportional to  $\kappa$  [15]. Choosing a suitable time scale the equation of continuity yields

$$U = \frac{\partial^2 \kappa}{\partial s^2}. \quad (4)$$

In fact, now the curves are characterized by their curvature [a set of  $\kappa_\alpha(s,t)$  functions] and the sign convention for  $\kappa$  is chosen to have positive curvature for a circular domain of the high-density phase.

It is worth mentioning that similar interfacial transport is taken into consideration for the surface evolution described by the conserved Kardar-Parisi-Zhang equation [13]. This description was proposed by Sun *et al.* [14] to study the dynamics of growing interfaces. In the former approach the interface is characterized by a height  $h(\mathbf{x},t)$  measured from a reference plane and  $h$  is assumed to be a single-valued function of position  $\mathbf{x}$ . Consequently, the former description does not allow us to study closed (or overhanging) curves and (generally) simplifies the effect of isotropic interfacial transport.

Many features of the motion of a closed curve have been well investigated previously [10–12]. Some quantities defined as integrals over the closed curve remain constant. For example, the tangent vector rotates  $\pm 2\pi$  along the curves, that is,

$$\int_0^{L_\alpha(t)} \kappa(s,t) ds = \pm 2\pi, \quad (5)$$

where  $L_\alpha(t)$  is the length of the given curve and the plus or minus sign indicates that the curve encloses a region of high or low concentration. As expected, the area is conserved for the dynamics given by Eq. (4) independently of whether it encloses a region of high or low concentration. This fact is in agreement with the particle-hole symmetry characterizing the systems we are interested in.

The time derivative of the length of a closed curve obeys the simple form

$$\frac{dL_\alpha}{dt} = \int_0^{L_\alpha(t)} \kappa_\alpha U ds = - \int_0^{L_\alpha(t)} \left( \frac{\partial \kappa_\alpha}{\partial s} \right)^2 ds. \quad (6)$$

According to this expression,  $L_\alpha(t)$  decreases monotonically and the single curve tends to form a circle conserving the initial area.

The domain structure observed during the critical coarsening is topologically similar to an ‘‘islands inside of lakes inside of islands . . .’’ pattern. When considering the corresponding set of curves one can observe the coalescence of

two curves (or domains). In the united curve immediately after the coalescence there appear two  $\pm \pi \delta(s-s_i)$  Dirac- $\delta$  peaks quickly spreading away. This process reduces the number of curves (domains) continuously and plays a crucial role in the formation of the domain structure. Henceforth we assume that the system evolves into the scaling regime for long times and the power-law behavior is maintained by the above processes.

In the scaling regime the time derivative of the total length of the curves may be written as

$$\frac{dL(t)}{dt} = \sum_\alpha \frac{dL_\alpha}{dt} = -AL(t), \quad (7)$$

where

$$A = \frac{1}{L} \sum_\alpha \int_0^{L_\alpha(t)} \left( \frac{\partial \kappa_\alpha}{\partial s} \right)^2 ds \quad (8)$$

denotes the average value of  $(\partial \kappa / \partial s)^2$  over all the curves. In the scaling regime the curvature varies typically from  $\pm 1/R(t)$  to  $\mp 1/R(t)$  in a length  $R$ . Consequently, the value of  $A$  may be approximated as

$$A \sim \frac{1}{R^4(t)}. \quad (9)$$

The total length  $L(t)$  is proportional to the total energy (measured from its asymptotic value) and is assumed to follow a power-law behavior for long times [16,4]. Substituting Eq. (9) into Eq. (7), this former power-law behavior can be satisfied if

$$R(t) \sim t^{1/4}, \quad (10)$$

in agreement with a previous prediction based on the field-theoretical analysis of the TDGL equation in the early stage of evolution [3].

In deriving the above result we have assumed that the material transport is localized along the interface and its strength is controlled by the variation of curvature. Although the real systems have enhanced interfacial conductivity, the mobile particles can leave the surface (evaporation) and these particles will give contribution to the bulk diffusion controlling the growth sooner or later. This picture implies that the dominance of interfacial conductivity may be prolonged by suppressing the rate of evaporation.

In order to check the above prediction the growth is studied with MC simulations in a half-filled, two-dimensional

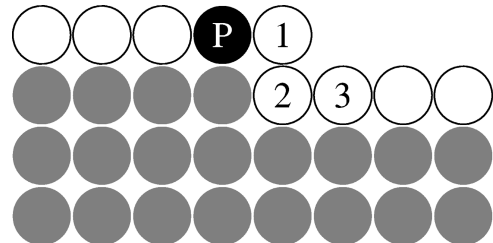


FIG. 1. Possible positions (open circles) for the mobile particle (black circle) walking through a step formed by other particles (gray circles).

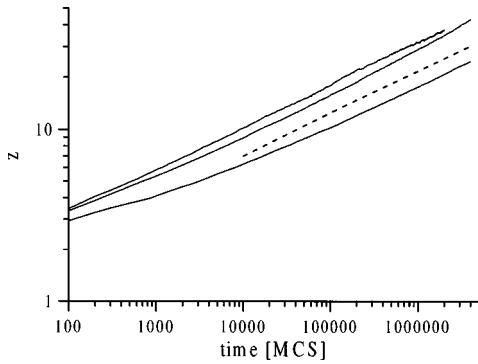


FIG. 2. Time dependence of the first zero of the pair correlation function for temperatures  $T=1.25$ , 1.0, and 0.5 (from top to bottom). The dashed line indicates a power-law behavior of  $t^{1/4}$ .

lattice-gas model choosing the attractive first- and second-neighbor interactions to be unity ( $J_1=J_2=1$ ). Because of the attractive interactions, this system decomposes into two phases below the critical temperature  $T_c=1.33(1)$  ( $k_B=1$ ). The evolution is governed by jumps of particles chosen randomly. In the present case the particle jumps to one of its first- and second-neighbor positions with a probability satisfying the condition of detailed balance (Kawasaki rate [17]). A similar model was used previously by Manna *et al.* [18] to investigate the effect of gravitation on the shape of drops sliding down on a wall and by Szabó *et al.* [19] to study the interfacial instability in a driven lattice gas.

The second-neighbor interactions and jumps are introduced to support the interfacial transport at the expense of bulk diffusion as demonstrated in Fig. 1. The mobile particle ( $P$ ) walking randomly along the curved interfaces should go over steps formed by the condensed particles. If only nearest-neighbor jumps are permitted, then the particle should stay on site 1, where it is bound to the interface by the second-neighbor interaction ( $J_2$ ). The attractive  $J_2$  prevents the particle from leaving the surface and from contributing to the bulk diffusion. Furthermore, the possibility of the second-neighbor jumps allows the particle  $P$  to jump directly to site 2. Notice that the jump from site 1 to 3 increases the role of interfacial diffusion too. All the above features together are responsible for the enhanced interfacial conductivity. Here it is worth mentioning that the second-neighbor interactions and jumps make the domain structure more isotropic.

The MC simulations are performed on a half-filled square lattice as large as  $1024 \times 1024$  under periodic boundary conditions. The system is started from a random distribution of particles. After a quench to a temperature  $T < T_c$ , the evolution of the domain structure has been monitored by evaluating the first zero of the pair-correlation function [ $C(z)=0$ ] characteristic of the typical domain size  $R(t)$  [4,9]. The domain size is determined as a function of time for times up to  $4 \times 10^6$  Monte Carlo steps (MCS) per particle.

Figure 2 shows the results on a log-log plot for three different temperatures. For  $T=1.25$  ( $T/T_c \approx 0.94$ ) the system evolves into the scaling regime after  $\sim 10^3$  MCS. Within this regime the correlation function satisfies the scaling ansatz reasonably well and  $R(t) \approx t^{1/4}$ . For lower temperatures the domain growth is slower and it requires much more time to reach the scaling regime.

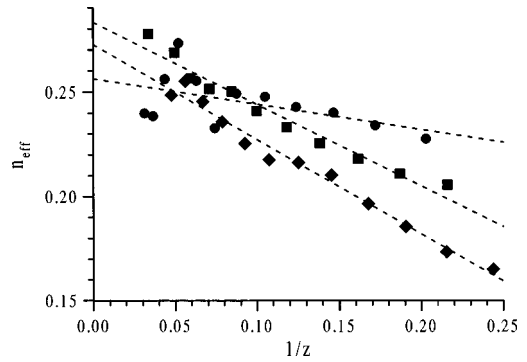


FIG. 3. Effective exponent vs  $1/z$  for  $T=1.25$  (circles), 1.0 (squares), and 0.5 (diamonds). The straight lines indicate the least-squares fits.

To study the convergence toward the asymptotic behavior we have also determined the effective exponent  $n_{eff}$  (the slope of curves in Fig. 2) [4,9]. Namely, we have fitted a power function to our data points between times  $t/2$  and  $2t$  and the exponent is plotted as a function of  $1/z(t)$ . The data plotted in Fig. 3 are averaged over two runs for the given temperatures (a single run of  $2 \times 10^6$  MCS takes a month on a Pentium processor). Very similar results are obtained when analyzing the time dependence of either the energy or the average domain size at low temperatures.

Figure 3 demonstrates that the MC data follow the law described by Eq. (1) and the  $y$  intercepts (extrapolated exponents) are sufficiently close to  $1/4$ . The best agreement has been observed for the highest temperature ( $T=0.94T_c$ ). In the vicinity of  $T_c$  Hume observed very similar behavior when studying the traditional lattice-gas model (with the nearest-neighbor interactions and jumps) for  $T=0.9T_c$  (see Fig. 4 in Ref. [9]). This result implies that the interfacial transport may play a dominant role for a sufficiently long period in the vicinity of  $T_c$  due to the wide and diffuse domain walls.

For lower temperatures ( $T=1$  and 0.5) the higher intercepts are caused by data of long times. This fact may be considered as an indication of the crossover to the  $t^{1/3}$  behavior. Despite this weak evidence I believe that the crossover should clearly appear for much longer times. For future simulations the crossover may be studied in models involving the second-neighbor interactions and jumps exclusively. As mentioned, the crossover was already observed by Puri and Oono [7] in a cellular dynamical system that takes the effect of second-neighbor cells into consideration too.

In summary, using two different methods I have studied the domain growth for a conserved order parameter when the critical coarsening is controlled by interfacial transport in a two-dimensional system. Accepting the scaling hypothesis, the geometrical approach gives direct evidence for the  $t^{1/4}$  growth law. The MC simulations confirm this asymptotic behavior for a wide range of time intervals when using a lattice-gas model having enhanced interfacial conductivity. Further systematic research is required to clarify how the bulk and interfacial transport can be modified by tuning the parameters of the lattice gases as well as to determine the crossover from the behavior of  $t^{1/4}$  to  $t^{1/3}$ .

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