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Cell-dynamics approach to late-stage domain growth in phase-separating systems

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The domain-growth problem in the kinetics of first-order phase transitions is studied by a computationally efficient discrete space-time model. The pair correlation function and the characteristic length scale are computed to a time regime which is about an order of magnitude later than in existing studies of the Langevin model. We find that the dynamical scaling function for the pair correlation function is identical to that found in studies of the Langevin model, and that the characteristic length scale satisfies the modified Lifshitz-Slyozov law of domain growth proposed for the kinetic Ising model. This indicates that these two models belong to the same dynamical universal class. No evidence is found to support the recent predictions of a $t^{1/4}$ growth law.

The purpose of this Rapid Communication is to examine the applicability of a recent novel approach by Oono and Puri[1] to the study of domain growth in problems involving the kinetics of first-order phase transitions. This "cell-dynamics" approach in principle provides an efficient algorithm for the numerical simulation of late-stage growth in systems such as binary alloys, but in our opinion has not yet been carried out for sufficiently long times necessary to establish the asymptotic behavior of their model. This is particularly worthwhile to establish, given the fact that a disagreement exists concerning the asymptotic growth law of the characteristic length scale [e.g., the linear domain size $R(t)$ with time t]. On the one hand, it has been suggested by Huse[2] that the asymptotic growth for the kinetic Ising model is described by a modified Lifshitz-Slyozov law $R(t) = At^{1/3} + B$ (where A and B are related to bulk and surface diffusion processes, respectively). It would appear that the argument of Ref. 2 would lead to a similar prediction for the Langevin model. On the other hand, a study involving renormalization-group ideas (together with numerical simulations) predicted[3] a power law $R \sim t^n$, with $n = \frac{1}{4}$ for the continuum Langevin model in two dimensions and claimed that these two models belonged to different dynamic universality classes.

Recent extensive Monte Carlo simulations[4,5] of the kinetic Ising model with a conserved order parameter show that the domain-growth law is in excellent agreement with the modified Lifshitz-Slyozov law.[6] Similar studies have been carried out quite recently for the continuum model by numerically integrating[7,8] the Lagevin equation. These studies also conclude that the asymptotic growth law is given by $n = \frac{1}{3}$ at late times, rather than the value $n = \frac{1}{4}$ predicted in the renormalization-group–type study. Clearly, as noted earlier, more work is needed to utilize the full potential of the cell-dynamics method, which by virtue of its efficiency might be able to clarify some of the important issues in the field of pattern formation.

In this paper we report some of the results of a numerical simulation of spinodal decomposition for the two-dimensional Langevin model, using the cell dynamics approach of Oono and Puri.[1] We consider a large lattice (256×256, which is at least four[1,7,8] and in some cases[3] 64 times the area of the lattice used by other authors) and carried out calculations for the pair correlation function for very late times. (This function was not computed by Oono and Puri.) Our work surpasses the original studies of Oono and Puri by about two orders of magnitude and obtains information about growth law and scaling behavior at times longer than considered in any other numerical study of continuum models, such as the Langevin or cell dynamics models. For example, the maximum value of the characteristic length in our study is about twice that calculated in recent simulations[7,8] of the Langevin model. This would imply that we are at a time which is at least 8 times larger than in the previous studies. Our main conclusions are the following: We find that dynamical scaling is satisfied for the pair correlation function in this model and that our data for the characteristic length scale is consistent with the modified Lifshitz-Slyozov law. No evidence of a $t^{1/4}$ growth law is found, which strongly suggests that the continuum Langevin (with a scalar order parameter) and kinetic Ising models belong to the same dynamical universal class.

In the Oono-Puri scheme, the original Langevin equation is replaced by the following equation:

$$\psi_i(t+1) = F[\psi_i(t)] - \langle\langle F[\psi_i(t)] - \psi_i \rangle\rangle \ , \qquad (1)$$

where

$$F[\psi_i(t)] = f[\psi_i(t)] + D[\langle\langle \psi_i(t) \rangle\rangle - \psi_i(t)] \ , \qquad (2)$$

$f(\psi) = A \tanh\psi$, D is a positive constant proportional to the phenomenological diffusion constant, and $\langle\langle\psi\rangle\rangle - \psi$ is essentially the isotropized discrete Laplacian $\nabla^2\psi$. We should note that we have considered for simplicity the zero-noise case, since there is by now considerable evidence to support the argument that the asymptotic domain growth law is independent of the noise.[7,8] Following Oono and Puri, we use the following definition of $\langle\langle\psi\rangle\rangle$

on the square lattice

$$\langle\langle\psi\rangle\rangle = \tfrac{1}{6}\sum\psi(\text{nearest-neighbor cells}) + \tfrac{1}{12}\sum\psi(\text{next-nearest-neighbor cells}) \ . \quad (3)$$

The motivation for replacing the Langevin equation by the cell dynamics in Eq. (1) is given in Ref. 1. In our numerical study, we have considered a square lattice of 256×256 points, with the order parameter ψ_i given at each of the lattice points. We have chosen $A=1.3$ and $D=0.5$, following Oono and Puri. Our initial distribution of ψ's is specified by a random, uniform distribution in the range $(-0.125, 0.125)$. To average over the initial distribution, we solved the equations a large number of times (70 "runs"). We have found that 70 runs is sufficient to yield accurate results, e.g., we estimate our error is within 1%–2%. We also made several long runs to very long times. The error bars associated with the quantities calculated in these runs are about 4%. Time is measured in number of updates per site. In this paper we have concentrated on the calculation of the correlation function $g(\mathbf{r},t)$, since it has been shown[2,7,8] that this yields a numerically accurate calculation of the characteristic length scale. The correlation function $g(r,t)$ was calculated from an average of $g(\mathbf{r},t)$ for $\mathbf{r}$ parallel to the lattice axes and lattice diagonals, respectively. The average characteristic length scale $R_g(t)$ is defined as the smallest value of r for which $g(r,t)=0$ at time t. The length $R_g(t)$ was calculated by fitting the four points in $g(r,t)$ closest to its first zero (of which two fall on each side of its first zero) to a cubic polynomial of r and defining $R_g(t)$ as the value of r where this fitted function vanishes. Our results for $R_g(t)$ are shown in Figs. 1 and 2. In Fig. 1 we plot $R_g(t)$ vs $t^{1/3}$ and in Fig. 2 we plot it against $t^{1/4}$. It is clear that $R_g=A+Bt^{1/3}$ is a much better representation of the data than either a $t^{1/4}$ growth[3] or a crossover from an early time $t^{1/4}$ behavior to a late time $t^{1/3}$ behavior.[1] The crossover time was estimated to be about 2000 updates/site for the zero noise case in the original study[1] which was based on the first moment of the structure function. However, our data seem to obey the $t^{1/3}$ law given above at a much earlier time and we do not observe any crossover behavior.

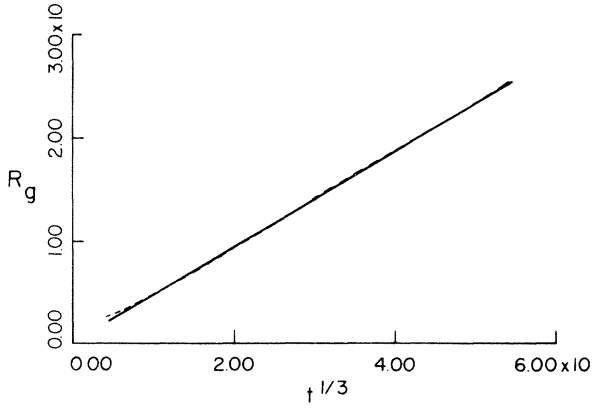

FIG. 1. Plot of our data for R_g vs $t^{1/3}$. The straight line is the best fit to the data.

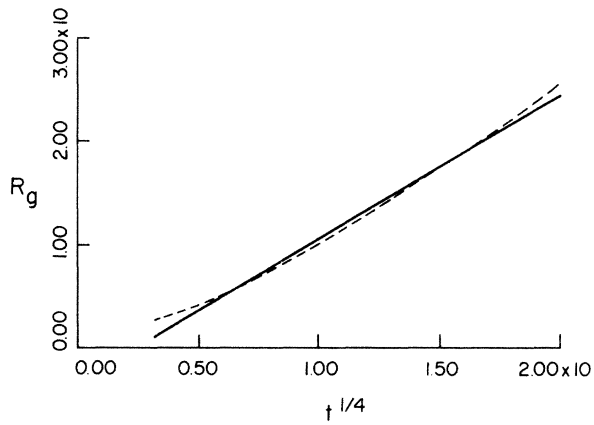

FIG. 2. Plot of R_g vs $t^{1/4}$. The straight line is the attempted fit to the data.

In order to analyze the data in an equivalent yet transparent manner, we define an effective exponent following Huse[2] as

$$n_{\text{eff}}(t) = \frac{d[\ln R_g(t)]}{d(\ln t)} \ . \quad (4)$$

Huse predicted that this quantity behaves at long times as

$$n_{\text{eff}}(t) = \tfrac{1}{3}\{1 - R_0/R_g(t) + O[R_g^{-2}(t)]\} \ , \quad (5)$$

where the length R_0 arises from surface diffusion effects. In Fig. 3 we plot $n_{\text{eff}}(t)$ vs $1/R_g(t)$ where we calculated $n_{\text{eff}}(t)$ as

$$n_{\text{eff}}(t) = \log_2[R_g(2t)/R_g(t)] \ . \quad (6)$$

As can be seen $n_{\text{eff}}(t)$ approaches $\frac{1}{3}$ as $1/R_g \to 0$, as expected in Eq. (5).

We also addressed the validity and extent of the dynamical scaling ansatz, which states that the pair correlation function satisfies a scaling relation $g(r,t)$

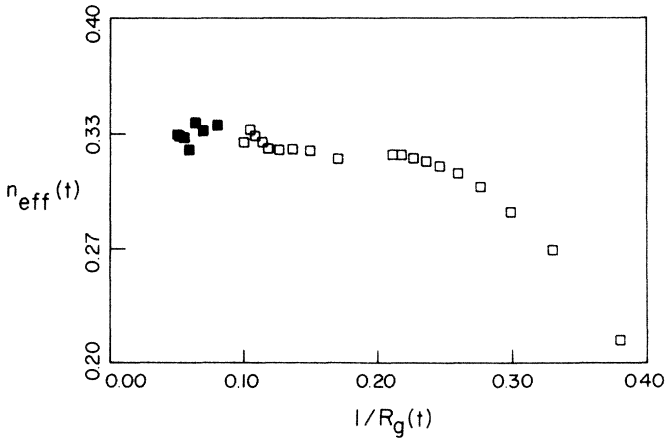

FIG. 3. Effective exponent $n_{\text{eff}}(t)$ [defined in Eq. (6)] vs $1/R_g(t)$. The open squares are computed from the data of $R_g(t)$ averaged over 70 runs. The solid squares belong to the late time data of $R_g(t)$ averaged over 5 runs.

$=f[r/R_g(t)]$ for t greater than some initial "transient" time t_0. In Fig. 4 we show the results by plotting $g(r,t)$ vs $r/R_g(t)$ for various values of t. It seems clear that the system is in the scaling regime for $t \geq 2000$, whereas, for earlier times systematic deviations from scaling are seen.[9] It is interesting to note that Oono and Puri claimed to see a growth law with exponent $\frac{1}{4}$ in this regime where actually the system is yet to enter the scaling regime. It is important to note that the characteristic length of Oono and Puri, defined as a moment of the structure factor, in general is a different physical length scale than our R_g. Thus, it is quite possible that before one enters the scaling regime the time dependence of these two lengths is different.

Perhaps the most important point beyond our result for the growth law is that the scaled form of $g(r,t)$ is *identical* to the scaling function calculated in recent simulations[7,8] of the Langevin equation for various values of the noise (including the zero noise considered here), at least for $r/R_g \leq 3.5$, over which one usually has numerically accurate data. It is of course also important to note that none of these studies can reveal whether or not scaling holds for large distances, at the largest times studied.

We conclude that dynamical scaling is obeyed in the model considered here at sufficiently late times. Our results strongly favor a modified Lifshitz-Slyozov growth law and imply that the Langevin model for scalar order parameter and spin-exchange kinetic Ising model belong to the same dynamic universality class. As well, cell dynamics seems to provide a very efficient approach to problems such as studied here.

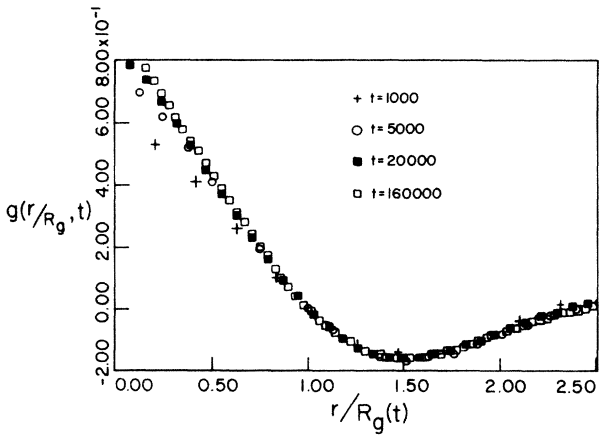

FIG. 4. Correlation function $g(r,t)$ at various times t vs scaled distance $r/R_g(t)$. Systematic deviations from scaling are observed at early times ($t < 2000$).

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[5]K. Kaski and J. D. Gunton (unpublished); J. D. Gunton, E. T. Gawlinski, and K. Kaski, in *Dynamics of Ordering Processes at a Phase Transition,* edited by S. Komura (Plenum, New York, in press).
[6]The authors of Ref. 3 originally proposed a $\ln t$-type growth law [see, for example, G. F. Mazenko, O. T. Valls, and F. C. Zhang, Phys. Rev. B **32**, 5807 (1985)] but have recently withdrawn their claim (Ref. 3) in view of the results in Ref. 4.
[7]E. T. Gawlinski, J. D. Gunton, and J. Viñals (unpublished).
[8]T. M. Rogers, K. R. Elder, and R. C. Desai (unpublished).
[9]We have found that $\langle \psi^2(t) \rangle$ approaches its asymptotic value very slowly with time in this model, as seen, for example, in Ref. 3. For this reason, we have computed a "normalized" correlation function $g_{\text{norm}}(r,t)$ which is $g(t,t)/\langle \psi^2(t) \rangle$, and checked its scaling behavior by plotting it against $r/R_g(t)$. $g_{\text{norm}}(r,t)$ scales in an equivalent way in the scaling regime.