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1990 J. Phys.: Condens. Matter 2 9215

(http://iopscience.iop.org/0953-8984/2/46/021)

J. Phys.: Condens. Matter **2** (1990) 9215–9220. Printed in the UK

LETTER TO THE EDITOR

A model simulation study of domain growth in a system with multiply degenerate ordered states

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Received 28 August 1990

Abstract. We study the dynamics of domain growth in a system with multiply degenerate ordered states. Using a phenomenological model recently proposed by us, we perform two-dimensional simulations to study the time-dependent behaviour of such degenerate systems. In the final stage the average size of the ordered domains is found to grow with time t as $t^{1/2}$, independently of the degeneracy p. The p-dependence of the asymptotic scaling functions for the domain size distribution is also discussed.

Recently the dynamics of ordering and coarsening processes in multiply degenerate systems has been attracting much interest [1–6]. For example, the time-dependent behaviour of order–disorder transitions of Cu_3Au [1, 2] and Ni_3Mn [3, 4] alloys has been investigated by various authors, using time resolved neutron or x-ray scattering techniques. In these systems, Au or Mn atoms occupy any of four equivalent sites for the FCC lattice. Therefore, the degeneracy of the ordered states is four. Recent experimental results for such degenerate systems confirm that three distinct physical regimes can be distinguished: nucleation, ordering, and coarsening. Initially the alloy is annealed at a high temperature in the disordered state, and at time $t = 0$ it is rapidly quenched to a fixed temperature below the ordering temperature. Clusters of the ordered phases then appear within a matrix of a disordered phase. The individual clusters may be in any of the p-allowed ordered states. As time goes by, the isolated cluster grows in size. This process may be termed ordering. Eventually the clusters meet each other, and the resulting system is composed of ordered domains in different ordered states, separated by domain walls. At this point the coarsening process begins, and the average size of ordered domains continues to grow. A similar process is observed in grain growth [7] and 2D soap froth [8, 9].

To study the growth kinetics of such degenerate systems, two different computational models have been proposed. One is the kinetic p-state Potts model [10], and the other is the vertex model [11, 12]. However, these models have been found to describe only the coarsening regime. Thus, we have recently proposed a model that can be used to distinguish the above time regimes [13]. This model is based on the time-dependent Ginzburg–Landau model [14] for the phase transition of superconductors, and is analogous to the model describing the commensurate–incommensurate transition [15]. In previous work [13] we have simulated the model to visualize typical evolution patterns.

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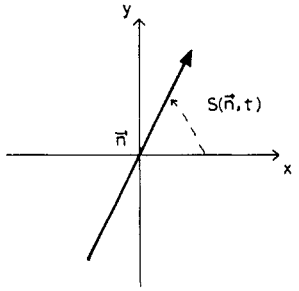

Figure 1. An arrow at lattice site $\boldsymbol{n}$ represents the phase variable $S(\boldsymbol{n}, t)$.

However, the simulations are still provisional as far as the time-dependent behaviour of the model is concerned. For reliable studies of the growth law of ordered phases, we simulate fairly large systems in 2D here.

In studying the dynamics of a system with spatial modulations, it is convenient to use a complex field, rather than a real one. Then, let $g(\boldsymbol{r}, t) \equiv F(\boldsymbol{r}, t) \exp(\mathrm{i}S(\boldsymbol{r}, t))$ be the complex scalar field at position $\boldsymbol{r}$ and time t. The amplitude $F(\boldsymbol{r}, t)$ of $g(\boldsymbol{r}, t)$ is positive valued and distinguishes stable ordered states from disordered ones, while the phase variable $S(\boldsymbol{r}, t)$ describes differences among the multiply degenerate ordered states. We assume that the equation describing the dynamics of the system considered here can be written as [13]:

$$\partial g(\boldsymbol{r}, t)/\partial t = -L\, \delta G[g]/\delta g^*(\boldsymbol{r}, t) \tag{1}$$

where L is a positive constant, the asterisk denotes the complex conjugate and the coarse-grained free energy $G[g]$ is a functional of $g(\boldsymbol{r}, t)$ and is taken to be

$$G[g] \equiv \int \mathrm{d}\boldsymbol{r}\, (\tfrac{1}{2}|\nabla g|^2 + W[g]) = \int \mathrm{d}\boldsymbol{r}\, (\tfrac{1}{2}|\nabla F|^2 + \tfrac{1}{2}F^2|\nabla S|^2 + W[g]) \tag{2}$$

with

$$\begin{aligned} W[g] &\equiv -|g|^2/2 + |g|^4/4 - (v/2p)(g^p + g^{*p}) \\ &= -F^2/2 + F^4/4 - (v/p)F^p \cos(pS) \end{aligned} \tag{3}$$

where p is a positive integer corresponding to the level of degeneracy of ordered states, and v is a positive constant.

After some algebraic calculations it is found that if $0 < v < A_p$, $W[g]$ has p-fold-degenerate minima at points (S_j, F_e), $j = 0, 1, \ldots, p-1$ with $S_j \equiv 2\pi j/p$ and $-1 + F_e^2 - vF_e^{p-2} = 0$. Here A_p is defined by

$$A_p = \begin{cases} [2/(p-4)][(p-2)/(p-4)]^{1-p/2} & \text{for } p > 4 \\ 1 & \text{for } p = 4 \\ \infty & \text{for } p = 2 \text{ and } 3. \end{cases} \tag{4}$$

This model is rather simplified, but is expected to capture the essence of the dynamical processes in a system with multiply degenerate ordered states. Note that in the present model, nucleation cannot be dealt with.

We solve equations (1)–(3) numerically, using the standard implicit formula, on an N^2 square lattice with periodic boundary conditions. The parameters are chosen to be $L = 0.01$, the time step $\Delta t = 1$, and the lattice spacing $\Delta x = \Delta y = 1$. Initially at each

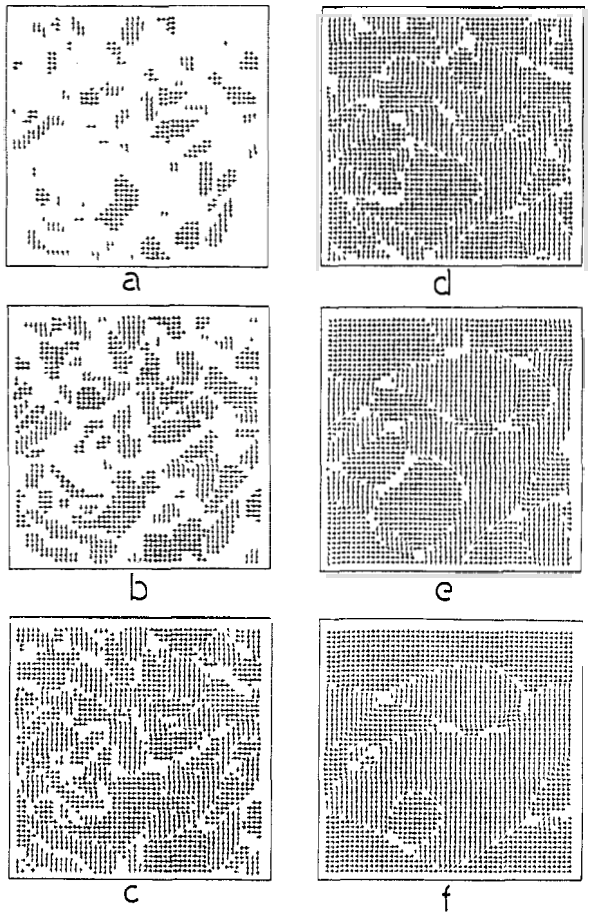

Figure 2. Time evolution of ordered regions for the case $p = 4$ at times (a) $t = 50$, (b) 100, (c) 500, (d) 10^3, (e) 5×10^3, (f) 10^4. Arrows are plotted at lattice sites satisfying $F(\boldsymbol{n}, t)/F_e > 0.9$ and $|S(\boldsymbol{n}, t) - j\pi/2| < \pi/16$ for $j = 0, 1, 2, 3$.

lattice site $\boldsymbol{n}$, $F(\boldsymbol{n}, 0)$ is chosen to be the positive value of a Gaussian random number with average 0 and variance 0.05, while $S(\boldsymbol{n}, 0) \bmod 2\pi$ is chosen to be a uniform random number in the interval $(-\pi, \pi)$. Note that we have examined other parameter values and the results below do not change qualitatively. For more details of the simulation method, see [13].

For the time being, we set $p = 4$ and $v = 0.1$. In figure 1 the ordered lattice site $\boldsymbol{n}$ is marked by an arrow. Here the ordered lattice site is characterized by the site with $F(\boldsymbol{n}, t)/F_e > 0.9$ and $|S(\boldsymbol{n}, t) - S_j| < \pi/4p$, $j = 0, 1, \ldots, p - 1$. In figure 2 the pattern evolution of the ordered regions is displayed on a 50^2 square lattice. From these figures we can see that four types of ordered cluster emerge and grow initially, and the larger domains coarsen at the expense of smaller ones in the final stage.

Now we discuss the time-dependent behaviour of the system. For this purpose we simulate the model using a 256^2 square lattice. Moreover, the following results are obtained by averaging over 50 independent simulation runs. In figure 3 we show the time evolution of the average size of ordered regions, $\bar{R}(t)$, defined by

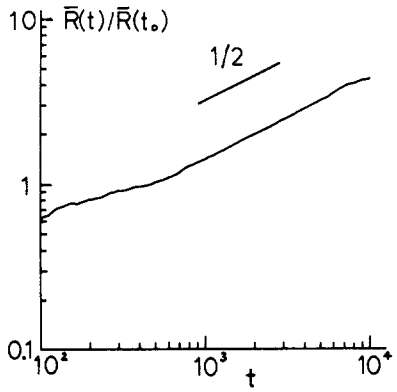

Figure 3. Time evolution of the average ordered domain size $[\bar{R}(t)/\bar{R}(t_0)]$, against t with $t_0 = 500$. A straight line is also shown with a slope indicated.

$$\bar{R}(t) \equiv \sqrt{\sum_i N_i(t)\,\Delta x\,\Delta y/n(t)}$$

where $N_i(t)$ is the number of lattice sites belonging to the ith ordered region and $n(t)$ is the total number of such ordered regions at time t. By the least squares method for 50 simulation data we obtain the growth exponent 0.48 ± 0.04 in the final stage. However, we cannot decide on the growth exponent in the early stages due to large statistical errors. Moreover, the $\frac{1}{2}$-power law is found to occur after a certain time t_0, where $\Sigma_i N_i(t_0) \simeq 256^2$. In the present case we find $t_0 \simeq 500$. Similar final-stage behaviour has been obtained numerically for the p-state Potts model [10] and the vertex model [11, 12]. On increasing the value of v in equation (3), vortex patterns often appear in the system, as was pointed out in [16]. Here vortices are characterized by regions with $F(\boldsymbol{n}, t)/F_e < 0.9$ in the final stage. This vortex formation, however, is found not to influence the growth law.

Next, to study the asymptotic behaviour of the system, we discuss the normalized distribution function $h(R, t)$ of domain size R. In figure 4 we show the normalized distribution function $H(x) \equiv \bar{R}(t)h(R, t)$ plotted against $x \equiv R/\bar{R}(t)$ for various times, satisfying

$$\int_0^\infty H(x)\,\mathrm{d}x = \int_0^\infty xH(x)\,\mathrm{d}x = 1.$$

From figure 4 we find that the distribution function reaches an asymptotic scaling function. Moreover, as was pointed out in the previous models [7, 9] the scaling function can be well approximated by the log–normal distribution function $f(x|\mu, \sigma)$ with two parameters μ and σ, given by

$$f(x|\mu, \sigma) = \begin{cases} (\sqrt{2\pi}\,\sigma x)^{-1} \exp[-(\ln(x) - \mu)^2/2\sigma^2] & \text{for } x > 0 \\ 0 & \text{for } x \leqslant 0. \end{cases} \tag{5}$$

In figure 4 the log–normal distribution function with two parameters $\sigma = 0.45$ and $\mu = -\sigma^2/2$ is represented as a full curve. Here the value of μ is chosen such that the first moment

$$\int_0^\infty xf(x|\mu, \sigma)\,\mathrm{d}x$$

is equal to one, while the value of σ is more or less arbitrary.

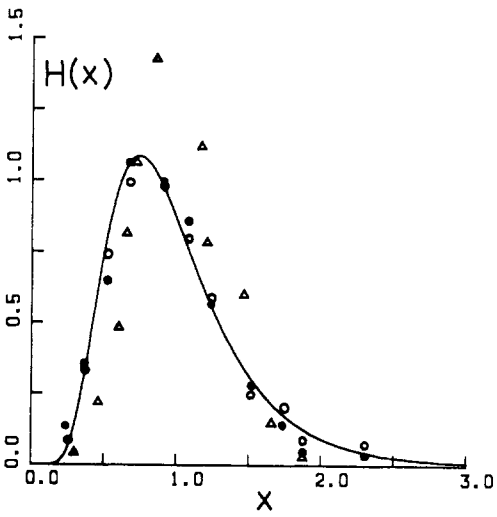

Figure 4. Normalized domain size distribution function $H(x)$ against $x \equiv R/\bar{R}(t)$ at times $t = 500$ (△), 10^3 (○) and 5×10^3 (●).

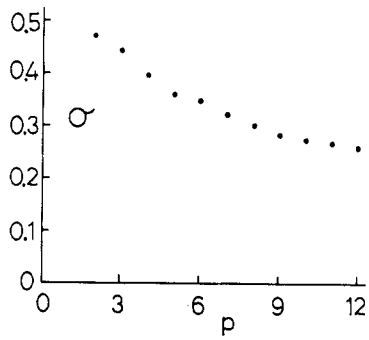

Figure 5. The parameter σ as a function of degeneracy p, which fits the simulation data well.

Finally we comment on the dependence on p- of the above results. We have simulated the model for $2 \leqslant p \leqslant 12$. From these simulation data the growth exponent in the final stages is found to be independent of the degeneracy p. However, the asymptotic scaling function for the domain size is found to depend on p, although the function of each value of p is well approximated by the log–normal distribution. In figure 5 we show the value of σ as a function of p, which fits the simulation data well. With increasing degeneracy p, the distribution function sharpens. This result is similar to that of the p-state Potts model [10].

In the present letter we have discussed the scaling function only for the domain size distribution in 2D. To check the validity of the present model, the scaling behaviour of the scattering structure factor will be discussed elsewhere. Moreover, the model in which equation (1) is replaced by

$$\partial g(\boldsymbol{r}, t)/\partial t = L\nabla^2 \, \delta G[g]/\delta g^*(\boldsymbol{r}, t) \tag{6}$$

is expected to describe the dynamical processes in multiply degenerate systems with conserved order parameter. The simulation of this modified model, as well as the 3D simulation, is now under way.

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