Morphology from the maximum entropy principle: Domains in a phase ordering system and a crack pattern in broken glass

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The maximum entropy principle is applied to study the morphology of a phase ordering two-dimensional system below the critical point. The distribution of domain area A is a function of ratio of the area to contour length L, $R=A/L(A)$, and is given by $\exp(-\lambda R^{\mu})$ with exponent $\mu=2$, which follows from the Lifshitz-Cahn-Allen theory. A and L are linked through the relation $L\sim A^{\nu}$. We find two types of domain in the system: large of elongated shape ($\nu=0.88$) and small of circular shape ($\nu=0.5$). A crack pattern in broken glass belongs to the same morphology class with $\mu=1$ and $\nu=0.72$.

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One of the main problems in statistical mechanics is the formulation of some general principles that govern the evolution of systems out of equilibrium. Here we show that for a system undergoing a phase transition one can use the maximum entropy principle [1] (MEP) to determine its morphology at each instant of time. As far as we know this is the first application of this principle to the kinetics of phase transitions [2]. Moreover, a *quantitative* analysis of system morphology allows us to determine the kinetic pathways along which the evolution of the system proceeds during the phase transition. In order to illustrate these ideas we study a symmetric two-dimensional (2D) system of the scalar nonconserved order parameter. Despite the fact that this simple system has been studied for almost 40 years [3], surprisingly, its morphology has not been determined *quantitatively* so far [2,4]. Although we get the morphology of this system from the maximum entropy principle we find that the dynamics of the system follows a kinetic pathway along which the dissipation (or production of entropy) is continuously reduced.

Cellular structures in 2D are known in many areas of science [5]. Whether we consider bee honeycomb, soap foam (or froth) [6–8], defect condensation of charge density waves [9], territory of fire ants [10], administrative divisions [11,12], superclusters of galaxies (large scale structure of the universe) [13], 2D sections of polycrystalline materials, chemical patterns on surfaces, or crack structure in ceramics [14], we find characteristic morphological patterns. Here we present a comparative study of a crack pattern in broken glass obtained in our experimental studies and the domain pattern of phase ordering systems in 2D obtained in our computer simulations. We find that these two different systems belong to the same morphological class. We are not aware of any previous studies of the morphology of the crack pattern in broken glass.

Computer simulations. The evolution of the 2D system with a scalar nonconserved order parameter below the critical point follows the dimensionless time dependent Landau-Ginzburg equation [2,4]:

$$\frac{\partial\phi(\mathbf{r},t)}{\partial t}=-\frac{\delta F[\phi]}{\delta\phi}, \tag{1}$$

where ϕ is the scalar order parameter, F is the Landau-Ginzburg free energy functional,

$$F[\phi]=\int d\mathbf{r}\left(\frac{1}{2}|\nabla\phi(\mathbf{r})|^2+f(\phi(\mathbf{r}))\right), \tag{2}$$

and $f(\phi)=-\phi^2/2+\phi^4/4$ is the bulk free energy. Equation (1) has been solved on square lattices of 512×512, 1024×1024, and 2048×2048 grid points with no apparent change of the results (except for very long times where finite size effects become apparent). The initial value of the field ϕ was chosen at each point of the lattice from a uniform distribution on $[-0.1,+0.1]$ with zero mean. In order to check the results for numerical artifacts we have varied the mesh size between $\Delta x=0.5$ and 2 and used four-and eight-point approximations for the Laplacian. We note that the statistical properties of the system, such as correlation function, size and shapes of the domains, growth laws, etc., do not depend on the initial distribution of the field ϕ after a few initial time steps of the evolution.

The initial pattern given by ϕ can be represented by the $+/-$ domains defined by the sign of ϕ. The system is symmetric under the change of sign $\phi\rightarrow-\phi$ and therefore the interface between $+/-$ domains is defined by $\phi(x,y)=0$. Since the system is simulated on a lattice the location of the interface is obtained by linear interpolation of ϕ between the lattice points. On Fig. 1 we show a typical snapshot of $(+/-)$ (black/white) domains in the late stage of the system evolution with sharp interfaces between the domains. The coarsening of the system (increase of the characteristic length scale) occurs via a change of shape of the irregular domains and the disappearance of smaller circular domains.

At the very beginning of the evolution the $(+/-)$ domains are very small. The dynamics is diffusive and mainly driven by the bulk free energy $f(\phi)$. After a few time steps the order parameter (initially close to zero) attains its bulk equilibrium value (saturation) inside the domains. In the process many small domains join together, forming larger domains with highly irregular shapes. Once the order parameter is saturated the character of the evolution changes from bulk driven to interface driven. The domains change their size and shapes by the movement of the interface. On the basis of Eq. (1) Lifshitz and Allen and Cahn [3] showed that the interface

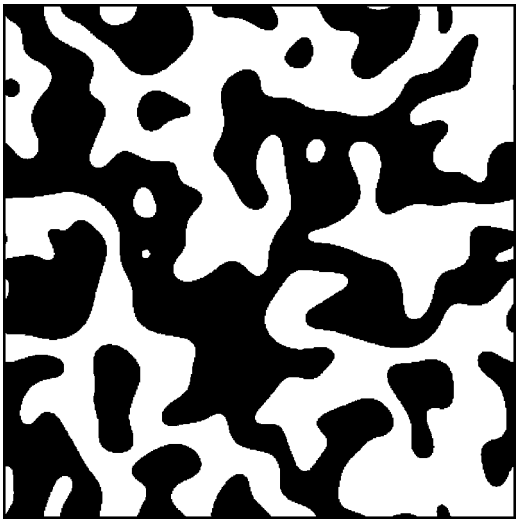

FIG. 1. Snapshot of the system during the late stages of evolution. The black domains correspond to $\phi(x,y)>0$ inside the domain and the white domains to $\phi(x,y)<0$. The domain interface is given by $\phi(x,y)=0$.

moves with velocity $v=-H$, where H is the local mean curvature. Assuming that the mean curvature is inversely proportional to the size of the domains $H\sim 1/R(t)$ the LCA theory predicts the growth law $R(t)=vt\sim t^{1/2}$, confirmed by computer simulations in the late stage of evolution [15].

The area and interface length distribution. In order to study the shapes of the domains we have triangulated them and computed for each domain its area A and length of interface L at each time step of the evolution. Next we computed the average values of their area and interface length $A_{\mathrm{av}}(t)$ and $L_{\mathrm{av}}(t)$, as a function of time. We found that the shape of the domains exhibits the following scaling relation:

$$L/L_{\mathrm{av}}(t)\sim(A/A_{\mathrm{av}}(t))^{\nu}, \tag{3}$$

where the exponent ν depends on whether the domain area A is above or below the average $A_{\mathrm{av}}(t)$:

$$\nu=\begin{cases}0.50\pm0.01 & \text{if } A<A_{\mathrm{av}}(t),\\ 0.88\pm0.02 & \text{if } A>A_{\mathrm{av}}(t).\end{cases} \tag{4}$$

This scaling relation is shown in Fig. 2, where we have taken all the domain areas and interface length for three different times ($t=400,500,1100$) and more than 330 000 domains. It is remarkable that all the domains for all times fall onto a single master curve, showing a high degree of regularity in the morphology of the system. In principle, for a highly irregular (chaotic) morphology we would see instead of a single curve many points scattered all over the diagram. This equation also shows that the system undergoing the phase ordering kinetics exhibits scaling at the level of the shapes of the domains. This means that the shapes of the domains at earlier times look statistically similar to the shapes at later times, apart from the global change of the average area and interface length.

It follows from Fig. 2 and Eq. (4) that in the late stage regime we find in the system two types of domain: large and

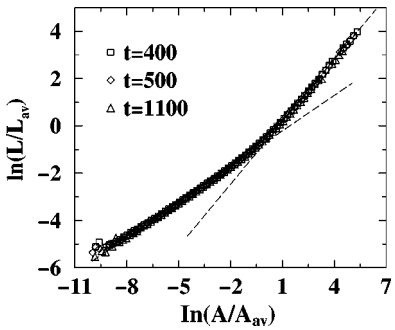

FIG. 2. The scaling relation between the interface length L and the domain (Fig. 1) area A during the process of phase ordering. Equations (3) and (4) are given by the dashed lines. On this plot we have put the results obtained for about 330 000 domains and three different times ($t=400,500,1100$). The master curve consists of two straight lines [Eqs. (3) and (4)], indicating two types of domain in the system.

elongated with contour length proportional (roughly) to their area ($L^{1/0.88}\sim A$) and circular domains for which $L^2\sim A$. The evolution follows a path along which the elongated domains change continuously into circular domains (Figs. 1 and 2). In this way dissipation is reduced. In order to see it let us consider the local energy change per unit time and unit length of the domain interface. This quantity is proportional to v^2 [2], where the local velocity of the interface $v=-H$. Integrating v^2 over the interface length of a domain gives the dissipation per domain. For a circular domain this dissipation is proportional to $1/L$ (since $H\sim 1/L$), while for the elongated domain it is $1/L^{0.14}$. Therefore the change of shape of the domains during this evolution follows a kinetic pathway along which the dissipation is continuously reduced.

Next we have determined the distribution of sizes of the domains, $p(A,t)$. Following the conjecture made by Jaynes [1] we assumed that the distribution can be obtained from the maximum entropy principle with some additional constraints. We have found that the entropy [1]

$$S(t)=-\int dA\, p(A,t)\ln p(A,t) \tag{5}$$

is maximized at each instant of time t subject to the condition

$$\int dA\, p(A,t)(A/L)^{\mu}=\text{fixed}, \tag{6}$$

where $\mu=2$ and the dependence of L on A, which reflects the system dynamics, is given by Eqs. (3) and (4). The exponent μ can be deduced from the LCA theory. Because $A/L\sim R(t)$ (domain size) we conclude that the condition (6) sets the characteristic time $\tau\sim[R(t)]^{\mu}\sim(A/L)^{\mu}$ proportional to the time needed to close the domain of size $R(t)$. From the LCA theory we have $\tau\sim R^2$ and consequently $\mu=2$. Similarly, for other systems undergoing phase transitions the exponent μ can be found from the growth of the average domain sizes. In this sense our analysis is robust and not restricted to the specific system under study.

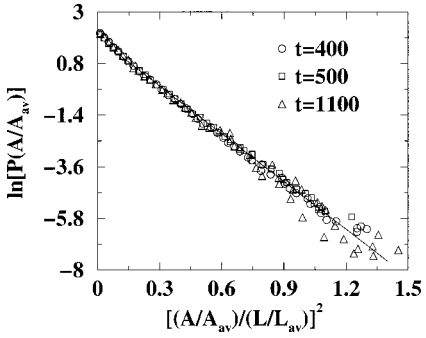

FIG. 3. The distribution function for the domain area in the late stage regime of the kinetics of a 2D system. It is shown in the scaled form $p(A,t) \sim \exp[-\alpha(x/y)^{\mu}]$ with $\mu=2$ $x=A/A_{\mathrm{av}}(t)$ and $y=L/L_{\mathrm{av}}(t)$ for three different times (see Fig. 2). Equation (8) is represented by the solid line. This fit strongly supports the MEP conjecture with the entropy $p(A,t)$ [Eq. (5)]. The distribution was obtained for about 330 000 domains.

From the maximization of $S(t)$ [Eq. (5)] subject to the constraint (6) we find

$$p(A,t)=C(t)\exp[-\lambda(t)(A/L)^{\mu}]. \tag{7}$$

Using the scaling principle we find the distribution in the rescaled form

$$p(x)=C^{*}\exp[-\lambda^{*}(x/y)^{\mu}], \tag{8}$$

where $x=A/A_{\mathrm{av}}(t)$, $y=L/L_{\mathrm{av}}(t)$, C^{*} and λ^{*} are constants independent of time, and $\mu=2$. Equation (8) is satisfied in the late stage regime as shown in Fig. 3, where the distribution $p(x)$ obtained from the simulations is plotted. This gives a strong support to the application of maximum entropy principle to the kinetics of the phase transition. Other distributions such as $p_1(L,t)$ can be obtained from $p(A,t)$ by a change of variables, i.e., $p_1(L,t)=p(A(L),t)dA(L)/dL$. We note that the choice of the distribution in Eq. (5) is not trivial. For example, a possible choice of $p_1(L,t)$ in Eq. (5) would lead to disagreement with our computer simulations.

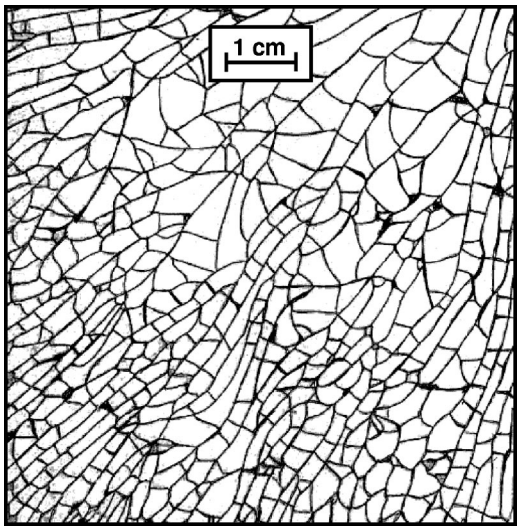

FIG. 4. Image of broken glass (a fragment) with a characteristic crack pattern.

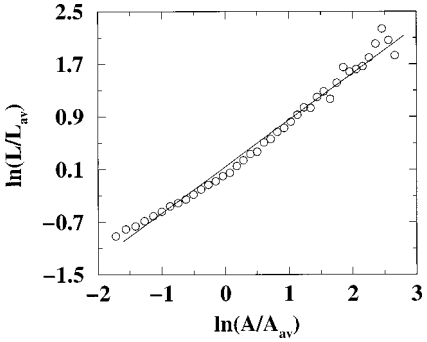

FIG. 5. The scaling relation between the contour length L of the domain boundaries and the area A for the crack pattern in broken glass (Fig. 4). Equation (3) with $\nu=0.72$ is given by the solid line.

The analysis presented here for the kinetics of phase transitions leads additionally to the definition of the 2D morphology class which can be characterized by two exponents (μ,ν). Equations (5) and (6) form the basis of the general principle which governs the form of the distribution function while Eqs. (3) and (4) are characteristic for a given system. There are other systems that belong to this class. One is the crack pattern in broken glass, discussed below, and another is the parcel division in towns mentioned in the conclusions. We are not aware of previous studies of these systems.

Crack pattern in a broken glass. The size of the hardened glass used in our experiment was approximately 1 m^2. The glass was broken and a crack pattern emerged (Fig. 4). The experiment was repeated with many samples of glass and for the morphological analysis we have used about 10^4 pieces of broken glass. In order to measure the area and boundary length of the glass pieces we put the broken glass on a transparency projector and made a photo of its image on a wall. Next we put the photo on a HP scanner and made an image in JPG format. Later, it was converted into a PPM format such that it allowed us to make a full analysis of the domains formed in this crack pattern. In Fig. 5 we show $y=L/L_{\mathrm{av}}$ versus $x=A/A_{\mathrm{av}}$ and find the same algebraic relation as in Eq. (3) with $\nu=0.72\pm0.02$. The area distribution $p(A)$ is obtained from the MEP principle with the constraint (6). We

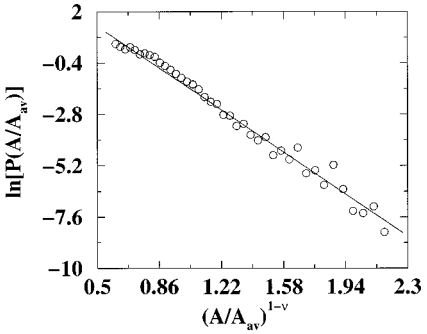

FIG. 6. The distribution function for the domain area in the crack pattern shown in Fig. 4. We find $p(A) \sim \exp[-\beta(x/y)^{\mu}]$ $(\mu=1)$ and since $y \sim x^{\nu}$ for all pieces of glass with $\nu=0.72$ we plot $p(A)$ in the rescaled form $\exp(-\beta x^{1-\nu})$.

find $p(A)$ for a broken glass pattern in the form of Eq. (8) with $\mu=1$. Condition (6) with $\mu=1$ expresses simply the fact that the characteristic domain size R_{char} of the crack pattern is fixed. Since the exponent ν in the relation $y\sim x^{\nu}$ is independent of the domain size, we have $p(A)=p(x)\sim\exp[-\beta(x/y)^{\mu}]\sim\exp(-\beta x^{1-\nu})$. In Fig. 6 we show the area distribution plotted as a function of $x^{1-\nu}$. This analysis shows that the crack pattern in broken glass belongs to the same morphology class as the domain pattern in a 2D system undergoing phase ordering.

Conclusions. Analysis based on the morphology of the system allows a detailed study of the kinetics of phase transitions. The phase transition as observed in time should follow a kinetic pathway in the direction of reduced dissipation. The maximum entropy principle is applicable to the analysis of 2D system morphology in phase ordering kinetics and the two exponents ν and μ can be used for its quantitative characterization. For systems undergoing phase transitions the constraint is imposed on the characteristic time of evolution and therefore the exponent μ should follow from the relation between the domain size and time. Unfortunately, not all 2D patterns follow such characterization. The soap froth show a different distribution of $p(A)$ since there are strong constraints imposed on their domain shape (e.g., a linear relation between the surface area and the number of sides of the cell [5]), which do not apply in the cases studied here.

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